

Examiner Habte,

I have searched this compound in two ways: by structure (see L32 for results), and by ring and elemental attributes, i.e., number of rings, ring systems, nitrogens, metals, etc., plus text (see L43 for results). For L43, I also used the priority date to limit results.

D que stat's are for both approaches are enclosed.

If you have any questions, please call me.

Thank you,

Mary Jane Ruhl
Ext. 22524

=> d his ful

FILE 'HCAPLUS' ENTERED AT 17:42:36 ON 02 APR 2004
L24 2 SEA ABB=ON L22 AND L23

FILE 'REGISTRY' ENTERED AT 17:49:32 ON 02 APR 2004
L25 STRUCTURE *see d que stat L32 for structure*
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L27 2079 SEA SSS FUL L25
L28 2 SEA ABB=ON L27 AND (FE OR MN OR CR OR RU OR CO OR CU OR NI)

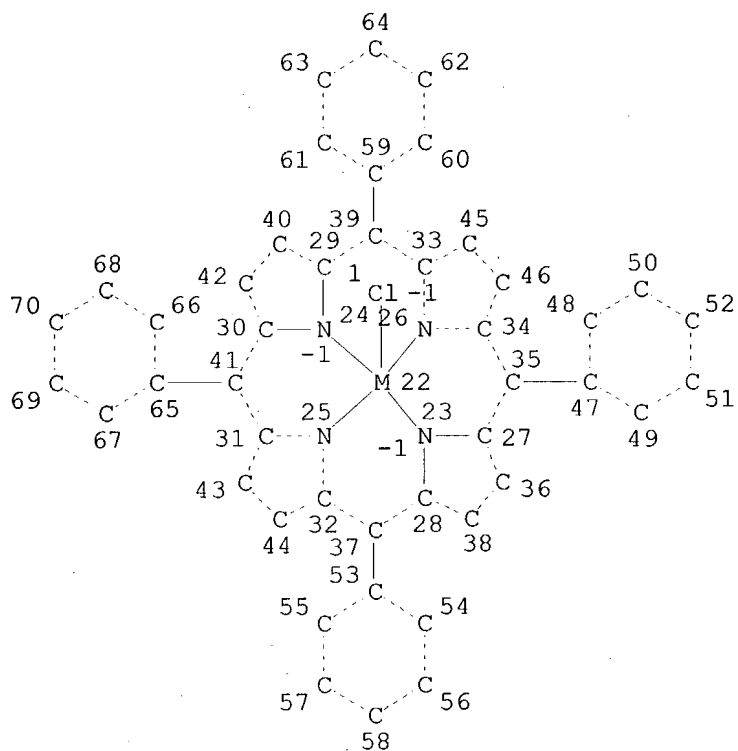
FILE 'HCAPLUS' ENTERED AT 17:56:39 ON 02 APR 2004
L29 6 SEA ABB=ON L28
L30 0 SEA ABB=ON L29 AND ?OXID?(W)?CATAL?
L31 0 SEA ABB=ON L29 AND ?CATAL?
L32 2 SEA ABB=ON L29 AND ?OXID? *2 hits in CAPLUS using structure +*
L33 0 SEA ABB=ON L29 AND ?EPOX? *text terms*
L34 0 SEA ABB=ON L29 AND (?DRUG? OR ?PHARM?) *See d que stat (attached)*

FILE 'REGISTRY' ENTERED AT 18:01:19 ON 02 APR 2004 *for L32*
L35 2 SEA ABB=ON L28 NOT CL
L36 18997 SEA ABB=ON NR=12 AND NRS=5
L37 8710 SEA ABB=ON L36 AND N=4
L38 49 SEA ABB=ON L37 AND (FE OR MN OR CR OR RU OR CO OR CU OR NI)

FILE 'HCAPLUS' ENTERED AT 18:04:50 ON 02 APR 2004
L39 1292 SEA ABB=ON L38
L40 126 SEA ABB=ON L39 AND ?OXID?(W)?CATAL?
L41 13 SEA ABB=ON L40 AND PRD<19990810 AND PD<19990810
SELECT RN L41 1-13

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=> d que stat l32
L25 STR



NODE ATTRIBUTES:

CHARGE IS E-1 AT 1
CHARGE IS E-1 AT 23
CHARGE IS E-1 AT 24
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 50

STEREO ATTRIBUTES: NONE

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L28 2 SEA FILE=REGISTRY ABB=ON L27 AND (FE OR MN OR CR OR RU OR CO
OR CU OR NI)
L29 6 SEA FILE=HCAPLUS ABB=ON L28
L32 2 SEA FILE=HCAPLUS ABB=ON L29 AND ?OXID?

=> d que stat 143

L36 18997 SEA FILE=REGISTRY ABB=ON NR=12 AND NRS=5
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L38 49 SEA FILE=REGISTRY ABB=ON L37 AND (FE OR MN OR CR OR RU OR CO
OR CU OR NI)
L39 1292 SEA FILE=HCAPLUS ABB=ON L38
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L43 13 SEA FILE=HCAPLUS ABB=ON L41 AND L42

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FILE 'HCAPLUS' ENTERED AT 18:07:22 ON 02 APR 2004

L43

13 SEA ABB=ON L41 AND L42

*13 hits in CAPLUS using
number of rings; modified
with metal ions + test tubes
See d que stat L43 (attached)*

=> d ibib abs hitstr 132 1-2

L32 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:569413 HCAPLUS

DOCUMENT NUMBER: 131:266166

TITLE: Structural characterization of bi-nuclear cobalt(III)
axial-methyl alcohol-hydrochloric acid
tetraphenyl-porphyrin complex

AUTHOR(S): Hashem, Khaled Mohamed Elewa; Hassan, Hamdi Ahmed;
Dayem, Hany Mohamed Abdel; Hassan, Salah Abdu

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Ain-Shams
University, Cairo, Egypt

SOURCE: Journal of Coordination Chemistry (1999), 48(3),
191-205

CODEN: JCCMBQ; ISSN: 0095-8972

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Simple modifications of the conventional preparation of Co(II)TPP led to a new Co complex. Structural study of the new complex was carried-out by using elemental anal., physicochem. and spectroscopic techniques. The EDXRF spectrum indicates Cl⁻ in 1:1 ratio with the Co ion. IR anal. indicates that (i) no changes in the main aromatic moieties of the ligand H₂TPP after chelation, (ii) the Co ion is sited in the porphyrin core, (iii) the O of MeOH is attached to a noncarbon atom, and (iv) Co-N bonds are coordinate bonds. UV results show a Co(III) metal ion is significantly changed by the nature of the axial ligands with only one band at 1525 nm. The split Soret band at 1395 and 1411 nm without shoulders could ensure the axiality of HCl and (HOMe) as electron withdrawing ligands. Measurement of the magnetic susceptibility indicates that +3 is the **oxidation** state of the central Co ion of the prepared complex. TGA anal. ensured that one Co(III) ion is chelated with one TPP²⁻ dianion to produce one mole of complex. XRD anal. reveals that the main porphyrin core is preserved. However, due to metalation, the length of the Co-Co bond in a binuclear structure, via lateral overlap of d_π-d_π orbitals to achieve back-donation, is estimated as 3.06-3.22 Å. NMR spectra of both H₂TPP and the prepared complex ensured removal of NH protons with characteristic bonds for both phenolic and pyrrolic protons. Although, the rotar protons of MeOH appear upfield, the HCl proton is assigned downfield. The number of protons detected by NMR is in agreement with that predicted by elemental anal. The final structure of the synthesized complex is predicted according to the C, H and N anal. as C₄₅H₃₃N₄OClCo in a binuclear form. The above anal. indicates that the binuclear structure is dominant in the solid phase; the charged structure is preferred in solution

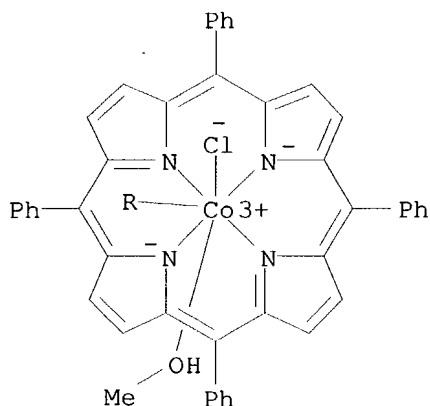
IT **245064-59-9P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure in solution)

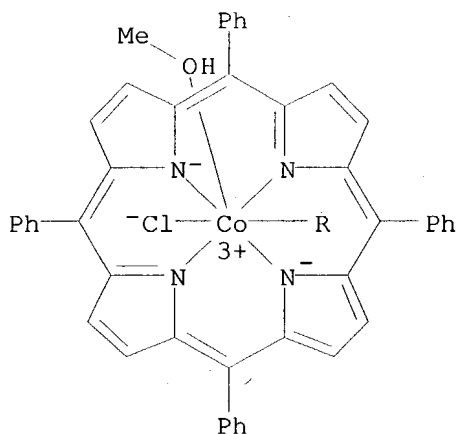
RN 245064-59-9 HCAPLUS

CN Cobalt, dichlorobis(methanol)bis[5,10,15,20-tetraphenyl-21H,23H-
porphinato(2-)-κN21,κN22,κN23,κN24]di-, (Co-Co)
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:113900 HCAPLUS

DOCUMENT NUMBER: 114:113900

TITLE: Studies on a tailed manganese porphyrin complex. (I). Preparation and the study of characteristics

AUTHOR(S): Shi, Tongshun; Chi, Xianglan; Wang, Qingming; Cao, Xizhang

CORPORATE SOURCE: Dep. Chem., Jilin Univ., Changchun, Peop. Rep. China

SOURCE: Wuji Huaxue Xuebao (1989), 5(4), 17-25

CODEN: WHUXEO; ISSN: 1001-4861

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB MnLC1 (H2L = meso-[o-(4-diethylamino)butyramidophenyl]triphenylporphyrin) was prepared and characterized by μ eff, cyclic voltammetry, and IR and electronic spectra. Adducts of both Mn(III) and Mn(II) complex with CO, NO, and organic bases were studied by spectroscopic method. Intramol.

coordination of the terminal Et₂N moiety was not observed in Mn(III) complex. The reduced form obtained from Mn(III) form exhibited electronic spectral characteristics of 5-coordinate Mn(II) complex.

IT **128086-52-2P**

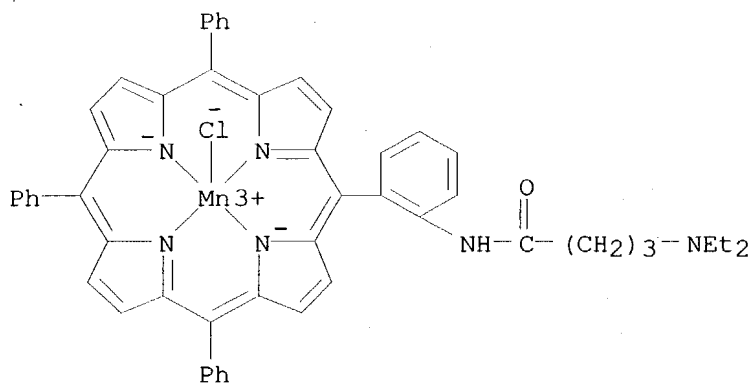
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and IR spectrum and cyclic voltammetry and reduction and reaction

of, with amines and nitric **oxide**)

RN 128086-52-2 HCAPLUS

CN Manganese, chloro[4-(diethylamino)-N-[2-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]butanamidato(2-)-N21,N22,N23,N24]-, (SP-5-13)- (9CI)
(CA INDEX NAME)



=> d ibib abs hitstr 143 1-13

L43 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:529154 HCAPLUS

DOCUMENT NUMBER: 131:144714

TITLE: Process for preparation of glyphosate by oxidizing
N-substituted glyphosates

INVENTOR(S): Morgenstern, David A.; Fobian, Yvette M.

PATENT ASSIGNEE(S): Monsanto Company, USA

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

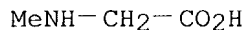
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| WO 9941260 | A1 | 19990819 | WO 1998-US2883 | 19980212 |
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| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9861663 | A1 | 19990830 | AU 1998-61663 | 19980212 <-- |
| AU 719152 | B2 | 20000504 | | |
| US 6005140 | A | 19991221 | US 1998-23404 | 19980212 <-- |
| NZ 335654 | A | 20000623 | NZ 1998-335654 | 19980212 <-- |
| EP 1062221 | A1 | 20001227 | EP 1998-906441 | 19980212 <-- |
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| RU 2184118 | C2 | 20020627 | RU 1999-109599 | 19980212 <-- |
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| TW 464537 | B | 20011121 | TW 1998-87102054 | 19980213 <-- |
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| MX 9904311 | A | 20000531 | MX 1999-4311 | 19990507 <-- |
| AU 728830 | B2 | 20010118 | AU 2000-17567 | 20000217 <-- |
| US 2001018536 | A1 | 20010830 | US 2001-776801 | 20010205 <-- |
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| | | | US 1998-22967 | A 19980212 <-- |
| | | | US 1998-23404 | A2 19980212 <-- |
| | | | WO 1998-US2883 | A 19980212 <-- |
| | | | US 1998-96207P | P 19980812 <-- |
| | | | US 1999-263171 | A3 19990305 <-- |

OTHER SOURCE(S): CASREACT 131:144714; MARPAT 131:144714

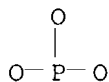
AB This invention is directed to process for preparation of R3OC(O)CH2NHCH2P(O)(OR4)(OR5) (R3, R4, R5 = independently H, substituted or unsubstituted hydrocarbyl, or an agronomically acceptable cation). The process comprises contacting a solution with a noble metal catalyst and introducing oxygen into the solution. The solution contains an N-substituted glyphosate R3OC(O)CH2N(CHR1R2)CH2P(O)(OR4)(OR5) (R1, R2 = independently H, halo, -PO3H2, -SO3H2, -NO2, (un)substituted hydrocarbyl other than -CO2H). This invention also relates to an **oxidation catalyst**

comprising a noble metal having a hydrophobic electroactive mol. species adsorbed thereon. Thus, reaction of sarcosine with phosphorus acid in HCl followed by treatment with formalin gave 70.5% N-methylglyphosate. Platinum catalyzed oxidative dealkylation of N-methylglyphosate in water in the presence of oxygen gave 85.4% glyphosate.

IT **107-97-1**, Sarcosine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphorylation of)
 RN 107-97-1 HCAPLUS
 CN Glycine, N-methyl- (9CI) (CA INDEX NAME)

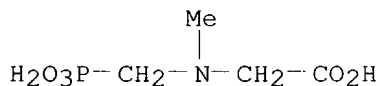


IT **13598-36-2**, Phosphorous acid, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphorylation of sarcosine with)
 RN 13598-36-2 HCAPLUS
 CN Phosphonic acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

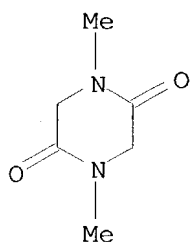


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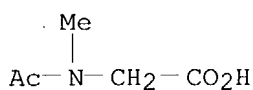
IT **24569-83-3P**, N-Methylglyphosate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and catalyzed oxidative dealkylation of)
 RN 24569-83-3 HCAPLUS
 CN Glycine, N-methyl-N-(phosphonomethyl)- (8CI, 9CI) (CA INDEX NAME)



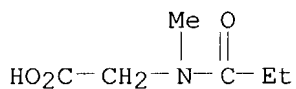
IT **5076-82-4**, Sarcosine anhydride **5888-91-5**,
 N-Acetylsarcosine **44897-56-5** **52558-39-1**
104608-53-9 **104766-31-6** **235755-16-5**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process for preparation of glyphosate by oxidizing N-substituted
 glyphosates)
 RN 5076-82-4 HCAPLUS
 CN 2,5-Piperazinedione, 1,4-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



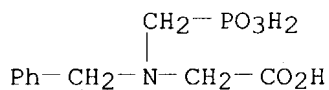
RN 5888-91-5 HCAPLUS
CN Glycine, N-acetyl-N-methyl- (9CI) (CA INDEX NAME)



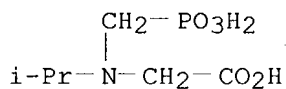
RN 44897-56-5 HCAPLUS
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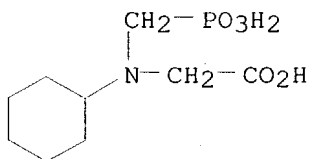
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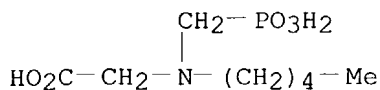
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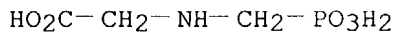
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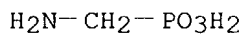
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CN Glycine, N-pentyl-N-(phosphonomethyl)- (9CI) (CA INDEX NAME)



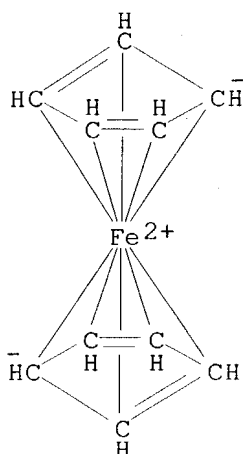
IT 1071-83-6P, Glyphosate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(process for preparation of glyphosate by oxidizing N-substituted
glyphosates)
RN 1071-83-6 HCAPLUS
CN Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



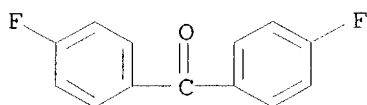
IT 1066-51-9P, AMPA
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of glyphosate by oxidizing N-substituted
glyphosates)
RN 1066-51-9 HCAPLUS
CN Phosphonic acid, (aminomethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



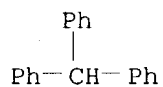
IT 102-54-5, Ferrocene 345-92-6, 4,4'-Difluorobenzophenone
519-73-3, Triphenylmethane 524-38-9,
N-Hydroxyphthalimide 2564-83-2, TEMPO 4316-58-9,
Tris(4-bromophenyl)amine 7061-81-6 7440-05-3,
Palladium, uses 7440-06-4, Platinum, uses 14172-92-0
14323-06-9 16456-81-8 36965-71-6
RL: CAT (Catalyst use); USES (Uses)
(process for preparation of glyphosate by oxidizing N-substituted
glyphosates catalyzed with)
RN 102-54-5 HCAPLUS
CN Ferrocene (8CI, 9CI) (CA INDEX NAME)



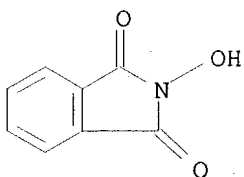
RN 345-92-6 HCAPLUS
CN Methanone, bis(4-fluorophenyl)- (9CI) (CA INDEX NAME)



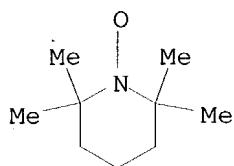
RN 519-73-3 HCAPLUS
CN Benzene, 1,1',1''-methyldynetrakis- (9CI) (CA INDEX NAME)



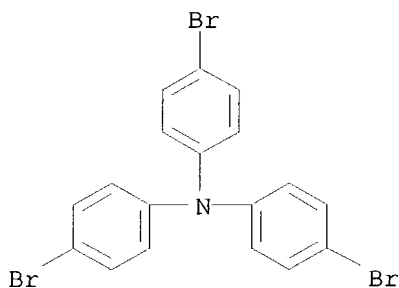
RN 524-38-9 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-hydroxy- (9CI) (CA INDEX NAME)



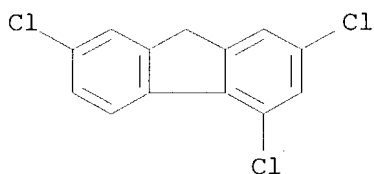
RN 2564-83-2 HCAPLUS
CN 1-Piperidinyloxy, 2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



RN 4316-58-9 HCAPLUS
CN Benzenamine, 4-bromo-N,N-bis(4-bromophenyl)- (9CI) (CA INDEX NAME)



RN 7061-81-6 HCAPLUS
CN 9H-Fluorene, 2,4,7-trichloro- (9CI) (CA INDEX NAME)



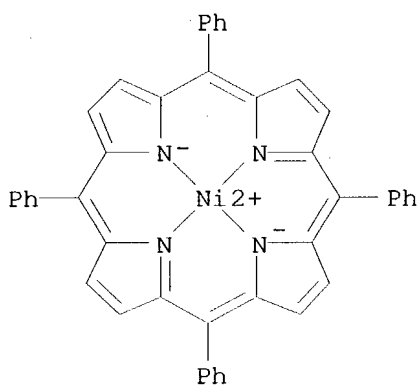
RN 7440-05-3 HCAPLUS
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

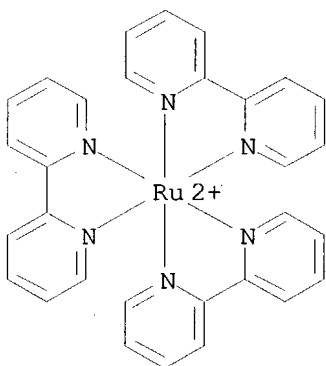
RN 7440-06-4 HCAPLUS
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

RN 14172-92-0 HCAPLUS
CN Nickel, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX
NAME)

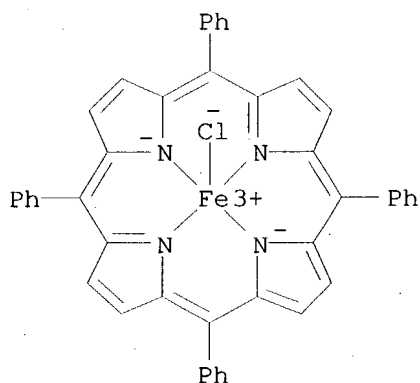


RN 14323-06-9 HCAPLUS
 CN Ruthenium(2+), tris(2,2'-bipyridine- κ N1, κ N1')-, dichloride,
 (OC-6-11)- (9CI) (CA INDEX NAME)

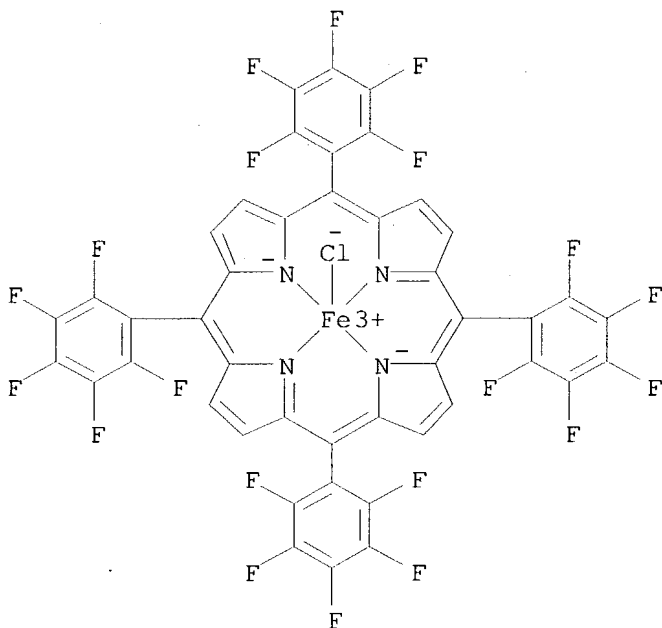


● 2 Cl⁻

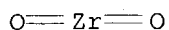
RN 16456-81-8 HCAPLUS
 CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-5-12)- (9CI) (CA INDEX
 NAME)



RN 36965-71-6 HCAPLUS
 CN Iron, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-5-12)- (9CI) (CA INDEX
 NAME)



IT 1314-23-4, Zirconium oxide, uses 1332-29-2, Tin oxide
 1344-28-1, Alumina, uses 7631-86-9, Silica, uses
 7727-43-7, Barium sulfate 13463-67-7, Titanium oxide,
 uses
 RL: CAT (Catalyst use); USES (Uses)
 (process for preparation of glyphosate by oxidizing N-substituted
 glyphosates catalyzed with platinum and)
 RN 1314-23-4 HCAPLUS
 CN Zirconium oxide (ZrO₂) (8CI, 9CI) (CA INDEX NAME)



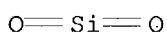
RN 1332-29-2 HCAPLUS
CN Tin oxide (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

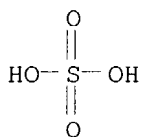
RN 1344-28-1 HCAPLUS
CN Aluminum oxide (Al₂O₃) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 7631-86-9 HCAPLUS
CN Silica (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

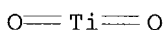


RN 7727-43-7 HCAPLUS
CN Sulfuric acid, barium salt (1:1) (8CI, 9CI) (CA INDEX NAME)



● Ba

RN 13463-67-7 HCAPLUS
CN Titanium oxide (TiO₂) (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L43 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:540887 HCAPLUS
DOCUMENT NUMBER: 119:140887
TITLE: Powders of cured resin compositions
INVENTOR(S): Kasamatsu, Haruo; Matsunaga, Fujinao; Kitano, Hisao
PATENT ASSIGNEE(S): Honshu Chemical Ind, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|--------------|
| JP 05097928 | A2 | 19930420 | JP 1991-155826 | 19910529 <-- |

PRIORITY APPLN. INFO.:

JP 1991-155826

19910529 <--

AB Mixts. of (A) oil-soluble phenol derivs. selected from catechol, resorcinol, biphenol, bicatechol, and biresorcinol, whose benzene rings contain unsatd. hydrocarbyl-containing substituents, and (B) polyfunctional unsatd. compds. containing aromatic rings are dispersed in H₂O as oil-drops or

emulsions

and polymerized oxidatively in the presence of Co compound catalysts to give title compns., useful for coatings, etc. Thus, blending Kuroiro Urushi (main component urushiol) 50, triallyl isocyanurate 3.3, and Co tetraphenylporphyrin 0.5 g at 30° gave an oily mixture, which was dispersed in an aqueous poly(vinyl alc.) containing NaCl, then an aqueous milk

casein

solution containing NaOH was added to the dispersion and the dispersion was stirred and blown with air to give microencapsulated cured powders.

IT 71-48-7, Cobalt acetate 814-89-1, Cobalt oxalate

932-69-4, Cobalt benzoate 1588-79-0 4486-50-4

5461-93-8 12672-51-4, Cobalt hydroxide

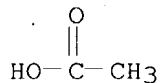
14172-90-8 26490-63-1 38150-63-9

RL: USES (Uses)

(catalysts., for oxidation polymerization of unsatd. phenol derivs. with aromatic unsatd. compds.)

RN 71-48-7 HCAPLUS

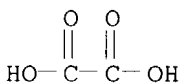
CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Co(II)

RN 814-89-1 HCAPLUS

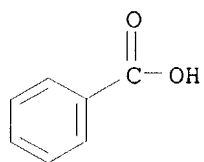
CN Ethanedioic acid, cobalt(2+) salt (1:1) (9CI) (CA INDEX NAME)



● Co(II)

RN 932-69-4 HCAPLUS

CN Benzoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Co(II)

RN 1588-79-0 HCAPLUS

CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

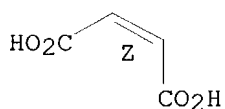
HO₂C- (CH₂)₆-Me

● 1/2 Co(II)

RN 4486-50-4 HCAPLUS

CN 2-Butenedioic acid (2Z)-, cobalt(2+) salt (1:1) (9CI) (CA INDEX NAME)

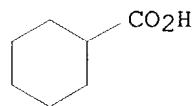
Double bond geometry as shown.



● Co(II)

RN 5461-93-8 HCAPLUS

CN Cyclohexanecarboxylic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Co(II)

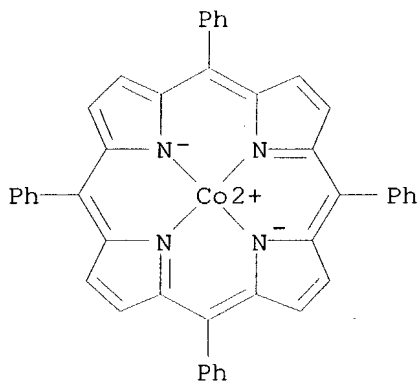
RN 12672-51-4 HCAPLUS

CN Cobalt hydroxide (9CI) (CA INDEX NAME)

| Component | Ratio | Component Registry Number |
|-----------|-------|------------------------------|
| HO | x | 14280-30-9 |

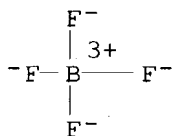
Co | x | 7440-48-4

RN 14172-90-8 HCAPLUS

CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
NAME)

RN 26490-63-1 HCAPLUS

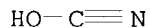
CN Borate(1-), tetrafluoro-, cobalt(2+) (2:1) (9CI) (CA INDEX NAME)



● 1/2 Co(II) 2+

RN 38150-63-9 HCAPLUS

CN Cyanic acid, cobalt(2+) salt (9CI) (CA INDEX NAME)



● 1/2 Co(II)

IT 149787-85-9P 149788-78-3P 149788-80-7P

149788-82-9P 149788-84-1P 149788-87-4P

149788-89-6P 149788-91-0P 149788-94-3P

149788-97-6P 149788-98-7P 149883-10-3P

149883-11-4P

RL: PREP (Preparation)

(preparation of, powdered, for coatings)

RN 149787-85-9 HCAPLUS

CN Urushiol, polymer with 1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-

trione (9CI) (CA INDEX NAME)

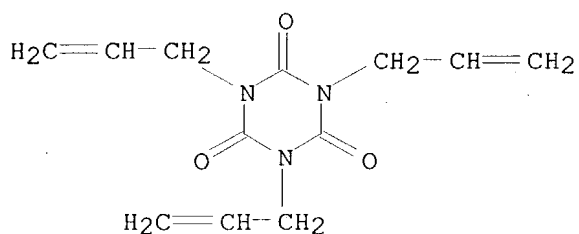
CM 1

CRN 53237-59-5
CMF Unspecified
CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

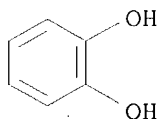
CRN 1025-15-6
CMF C12 H15 N3 O3



RN 149788-78-3 HCAPLUS
CN 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl-, polymer with (Z)-(9-octadecenyl)-1,2-benzenediol (9CI) (CA INDEX NAME)

CM 1

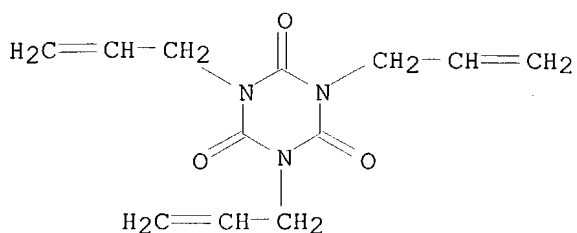
CRN 149788-77-2
CMF C24 H40 O2
CCI IDS



D1-(CH₂)₈-CH=CH-(CH₂)₇-Me

CM 2

CRN 1025-15-6
CMF C12 H15 N3 O3



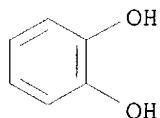
RN 149788-80-7 HCAPLUS
 CN 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(1-methylethyl)-, polymer with (Z,Z)-(9,12-octadecadienyl)-1,2-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 149788-79-4

CMF C24 H38 O2

CCI IDS

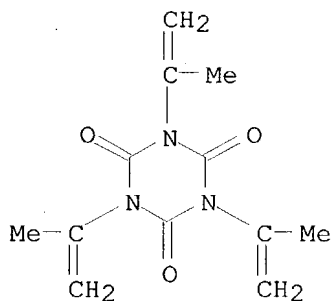


D1- (CH₂)₈-CH=CH-CH₂-CH=CH-(CH₂)₄-Me

CM 2

CRN 24468-25-5

CMF C12 H15 N3 O3



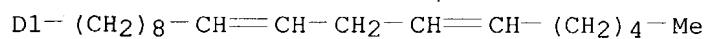
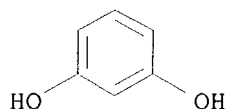
RN 149788-82-9 HCAPLUS
 CN 1,3-Benzenediol, (9,12-octadecadienyl)-, (Z,Z)-, polymer with diethenylpyridine (9CI) (CA INDEX NAME)

CM 1

CRN 149788-81-8

CMF C24 H38 O2

CCI IDS

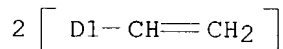
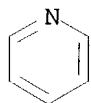


CM 2

CRN 26569-57-3

CMF C9 H9 N

CCI IDS



RN 149788-84-1 HCAPLUS

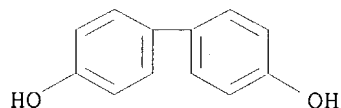
CN [1,1'-Biphenyl]-4,4'-diol, (9-octadecenyl)-, (Z)-, polymer with diethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 149788-93-2

CMF C30 H44 O2

CCI IDS

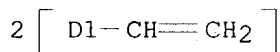


CM 2

CRN 1321-74-0

CMF C10 H10

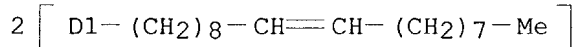
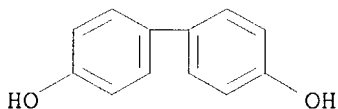
CCI IDS



RN 149788-87-4 HCAPLUS
 CN [1,1'-Biphenyl]-4,4'-diol, ar,ar'-di-9-octadecenyl-, (Z,Z)-, polymer with bis(1-methylethenyl)naphthalene (9CI) (CA INDEX NAME)

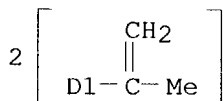
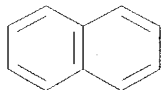
CM 1

CRN 149788-92-1
 CMF C48 H78 O2
 CCI IDS



CM 2

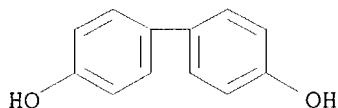
CRN 149788-85-2
 CMF C16 H16
 CCI IDS



RN 149788-89-6 HCAPLUS
 CN 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl-, polymer with 9,12-octadecadienyl[1,1'-biphenyl]-4,4'-diol and 2,4,6-tris(2-propenyloxy)-1,3,5-triazine (9CI) (CA INDEX NAME)

CM 1

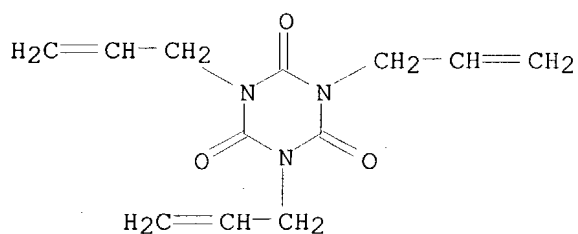
CRN 149788-88-5
 CMF C30 H42 O2
 CCI IDS



D1- (CH₂)₈-CH=CH-CH₂-CH=CH-(CH₂)₄-Me

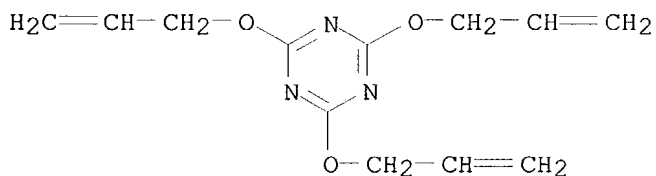
CM 2

CRN 1025-15-6
 CMF C12 H15 N3 O3



CM 3

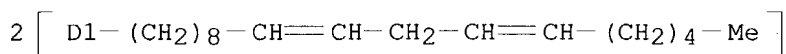
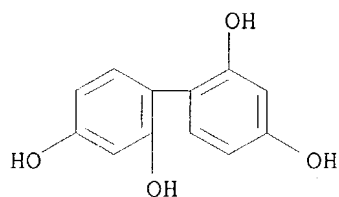
CRN 101-37-1
 CMF C12 H15 N3 O3



RN 149788-91-0 HCAPLUS
 CN 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2-methyl-2-propenyl)-,
 polymer with (all-Z)-ar,ar'-di-9,12-octadecadienyl[1,1'-biphenyl]-
 2,2',4,4'-tetrol (9CI) (CA INDEX NAME)

CM 1

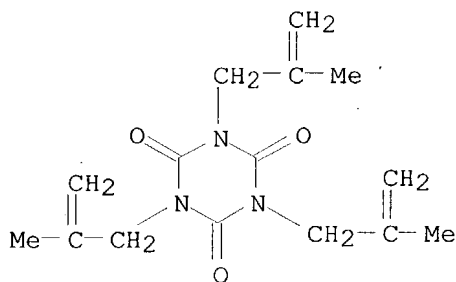
CRN 149788-90-9
 CMF C48 H74 O4
 CCI IDS



CM 2

CRN 6291-95-8

CMF C15 H21 N3 O3



RN 149788-94-3 HCAPLUS

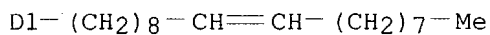
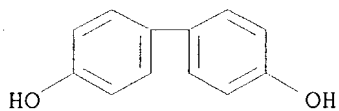
CN. [1,1'-Biphenyl]-4,4'-diol, ar,ar'-di-9-octadecenyl-, (Z,Z)-, polymer with (Z)-(9-octadecenyl)[1,1'-biphenyl]-4,4'-diol and 2,4,6-tris(2-propenyloxy)-1,3,5-triazine (9CI) (CA INDEX NAME)

CM 1

CRN 149788-93-2

CMF C30 H44 O2

CCI IDS

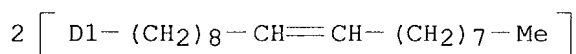
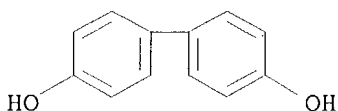


CM 2

CRN 149788-92-1

CMF C48 H78 O2

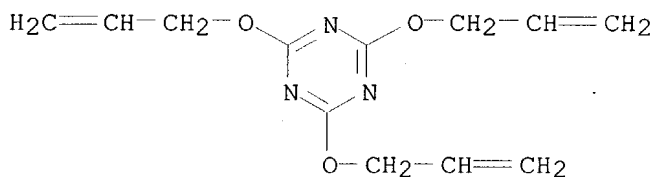
CCI IDS



CM 3

CRN 101-37-1

CMF C12 H15 N3 O3



RN 149788-97-6 HCAPLUS

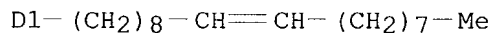
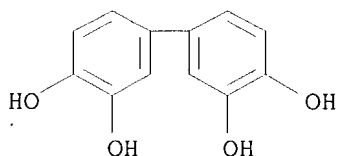
CN [1,1'-Biphenyl]-3,3',4,4'-tetrol, ar,ar'-di-9-octadecenyl-, (Z,Z)-, polymer with bis(1-methylethenyl)benzene, (Z)-(9-octadecenyl)[1,1'-biphenyl]-3,3',4,4'-tetrol and 2,4,6-tris(2-propenyloxy)-1,3,5-triazine (9CI) (CA INDEX NAME)

CM 1

CRN 149788-96-5

CMF C30 H44 O4

CCI IDS

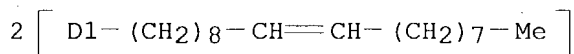
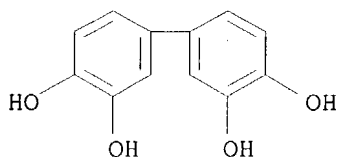


CM 2

CRN 149788-95-4

CMF C48 H78 O4

CCI IDS

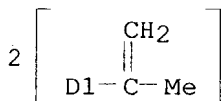


CM 3

CRN 27342-70-7

CMF C12 H14

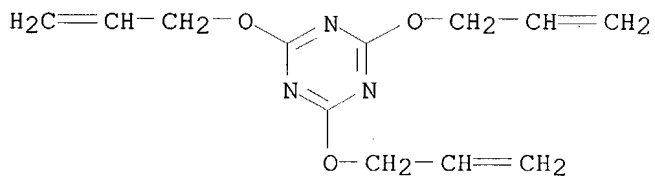
CCI IDS



CM 4

CRN 101-37-1

CMF C12 H15 N3 O3



RN 149788-98-7 HCAPLUS

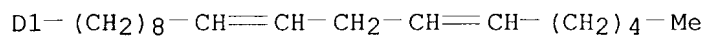
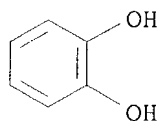
CN 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl-, polymer with diethenylbenzene and 9,12-octadecadienyl-1,2-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 149788-79-4

CMF C24 H38 O2

CCI IDS

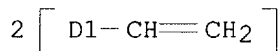


CM 2

CRN 1321-74-0

CMF C10 H10

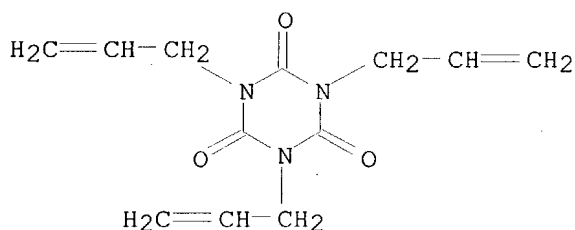
CCI IDS



CM 3

CRN 1025-15-6

CMF C12 H15 N3 O3



RN 149883-10-3 HCAPLUS

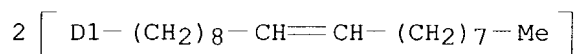
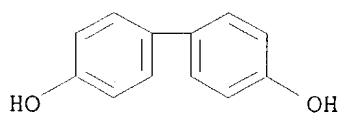
CN Urushiol, polymer with ar,ar'-di-9-octadecenyl[1,1'-biphenyl]-4,4'-diol, 1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione and 2,4,6-tris(2-propenyloxy)-1,3,5-triazine (9CI) (CA INDEX NAME)

CM 1

CRN 149788-92-1

CMF C48 H78 O2

CCI IDS



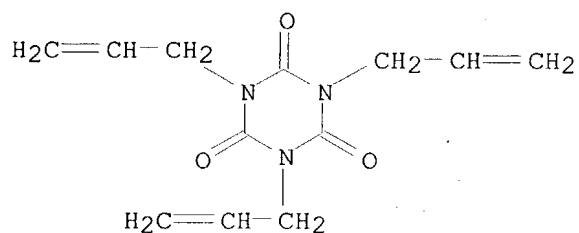
CM 2

CRN 53237-59-5
CMF Unspecified
CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

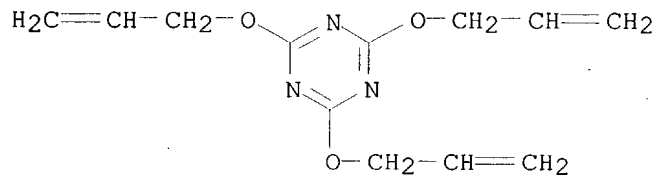
CM 3

CRN 1025-15-6
CMF C12 H15 N3 O3



CM 4

CRN 101-37-1
CMF C12 H15 N3 O3

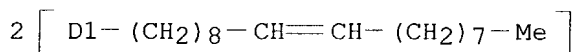
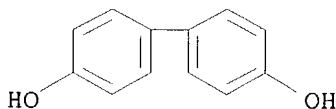


RN 149883-11-4 HCAPLUS
CN [1,1'-Biphenyl]-4,4'-diol, ar,ar'-di-9-octadecenyl-, (Z,Z)-, polymer with diethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 149788-92-1
CMF C48 H78 O2

CCI IDS

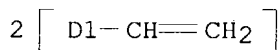


CM 2

CRN 1321-74-0

CMF C10 H10

CCI IDS



L43 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:494707 HCAPLUS

DOCUMENT NUMBER: 119:94707

TITLE: Processes for producing carbamates and isocyanates

INVENTOR(S): Leung, Tak W.; Dombek, Bernard D.

PATENT ASSIGNEE(S): Union Carbide Chemicals and Plastics Technology Corp.,
USA

SOURCE: U.S., 13 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

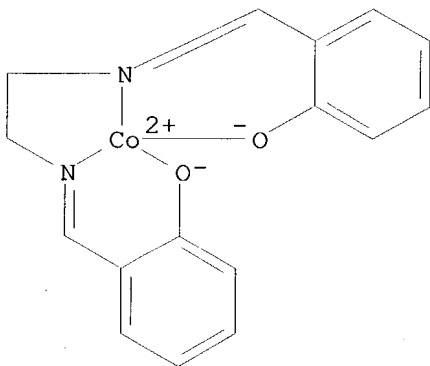
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| US 5194660 | A | 19930316 | US 1990-631962 | 19901221 <-- |
| PRIORITY APPLN. INFO.: | | | US 1990-631962 | 19901221 <-- |

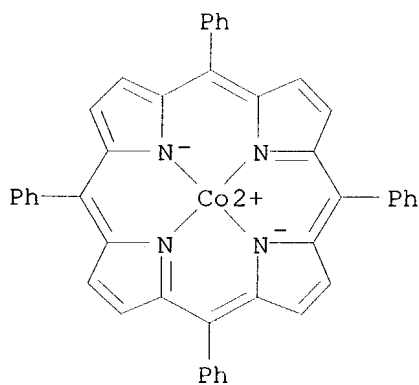
OTHER SOURCE(S): CASREACT 119:94707

AB Carbamates are prepared by oxidative carbonylation of primary or secondary amines or ureas with CO in presence of an alc., an O-containing oxidizing agent, metalloporphyrin or metal phthalocyanine catalyst derived from Group IIIa-Va and Group VIII metals, and an iodine-containing promoter. Decomposition of carbamates prepared in this manner affords isocyanates. Thus, reaction of 3.0 g tert-BuNH₂, 0.20 g CoPc (Pc = phthalocyanine dianion), and 1.0 g NaI with 40 g EtOH under 80 psi O₂/1520 psi CO afforded 99%

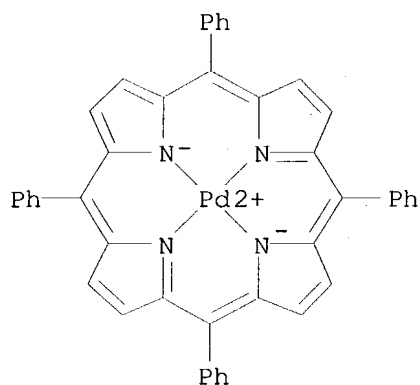
yield of Et N-tert-Bu carbamate.
 IT 14167-18-1 14172-90-8 14187-13-4
 21519-18-6 28903-71-1 58482-09-0
 77944-60-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, promoted with alkali metal iodide, for oxidative
 carbonylation of amine with carbon monoxide in presence of alc.)
 RN 14167-18-1 HCAPLUS
 CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[pheno
 lato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



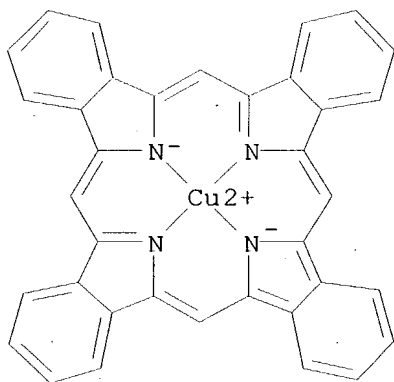
RN 14172-90-8 HCAPLUS
 CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κN21,κN22,κN23,κN24]]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



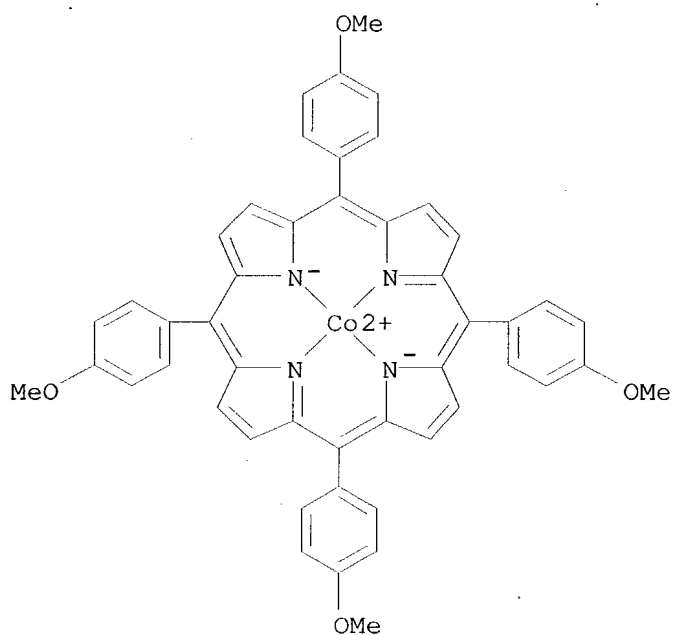
RN 14187-13-4 HCAPLUS
 CN Palladium, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κN21,κN22,κN23,κN24]]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



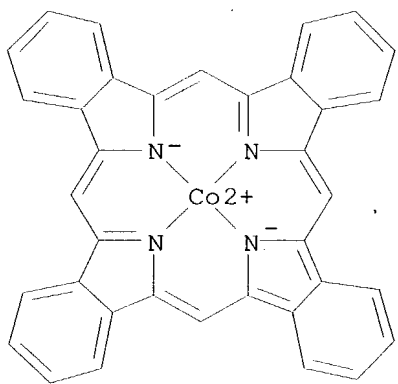
RN 21519-18-6 HCAPLUS
 CN Copper, [29H,31H-tetrabenzob[b,g,l,q]porphinato(2-)-
 κ N29, κ N30, κ N31, κ N32]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



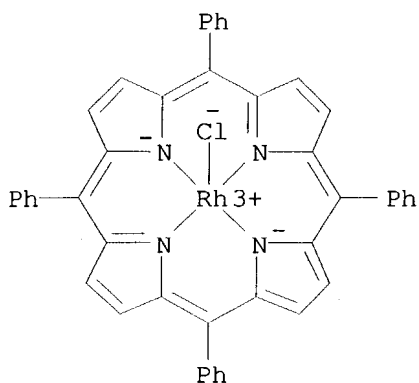
RN 28903-71-1 HCAPLUS
 CN Cobalt, [5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



RN 58482-09-0 HCAPLUS
 CN Cobalt, [29H,31H-tetrabenzo[b,g,l,q]porphinato(2-)-
 κN29,κN30,κN31,κN32]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



RN 77944-60-6 HCAPLUS
 CN Rhodium, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX
 NAME)



IT 7439-89-6D, Iron, metalloporphyrin complexes 7439-96-5D, Manganese, metalloporphyrin complexes 7439-97-6D, Mercury, metalloporphyrin complexes 7439-98-7D, Molybdenum, metalloporphyrin complexes 7440-02-0D, Nickel, metalloporphyrin complexes 7440-05-3D, Palladium, metalloporphyrin complexes 7440-16-6D, Rhodium, metalloporphyrin complexes 7440-28-0D, Thallium, metalloporphyrin complexes 7440-31-5D, Tin, metalloporphyrin complexes 7440-32-6D, Titanium, metalloporphyrin complexes 7440-33-7D, Tungsten, metalloporphyrin complexes 7440-36-0D, Antimony, metalloporphyrin complexes 7440-38-2D, Arsenic, metalloporphyrin complexes 7440-47-3D, Chromium, metalloporphyrin complexes 7440-48-4D, Cobalt, metalloporphyrin complexes 7440-50-8D, Copper, metalloporphyrin complexes 7440-62-2D, Vanadium, metalloporphyrin complexes 7440-66-6D, Zinc, metalloporphyrin complexes 7440-69-9D, Bismuth, metalloporphyrin complexes
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, promoted with iodine compound, for oxidative carbonylation of amines with carbon monoxide in presence of alc.)

RN 7439-89-6 HCAPLUS
 CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)

Fe

RN 7439-96-5 HCAPLUS
 CN Manganese (8CI, 9CI) (CA INDEX NAME)

Mn

RN 7439-97-6 HCAPLUS
 CN Mercury (8CI, 9CI) (CA INDEX NAME)

Hg

RN 7439-98-7 HCAPLUS
 CN Molybdenum (8CI, 9CI) (CA INDEX NAME)

Mo

RN 7440-02-0 HCAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-05-3 HCAPLUS
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-16-6 HCAPLUS
CN Rhodium (8CI, 9CI) (CA INDEX NAME)

Rh

RN 7440-28-0 HCAPLUS
CN Thallium (8CI, 9CI) (CA INDEX NAME)

Tl

RN 7440-31-5 HCAPLUS
CN Tin (8CI, 9CI) (CA INDEX NAME)

Sn

RN 7440-32-6 HCAPLUS
CN Titanium (8CI, 9CI) (CA INDEX NAME)

Ti

RN 7440-33-7 HCAPLUS
CN Tungsten (8CI, 9CI) (CA INDEX NAME)

W

RN 7440-36-0 HCAPLUS
CN Antimony (8CI, 9CI) (CA INDEX NAME)

Sb

RN 7440-38-2 HCAPLUS
CN Arsenic (7CI, 8CI, 9CI) (CA INDEX NAME)

As

RN 7440-47-3 HCAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7440-48-4 HCAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

RN 7440-50-8 HCAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

RN 7440-62-2 HCAPLUS
CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

RN 7440-66-6 HCAPLUS
CN Zinc (7CI, 8CI, 9CI) (CA INDEX NAME)

Zn

RN 7440-69-9 HCAPLUS
CN Bismuth (7CI, 8CI, 9CI) (CA INDEX NAME)

Bi

IT 7647-15-6, Sodium bromide, uses 7681-11-0, Potassium
iodide, uses 7681-82-5, Sodium iodide, uses
RL: USES (Uses)
(metalloporphyrin catalysts promoted with, for oxidative carbonylation
of amines with carbon monoxide in presence of alc.)
RN 7647-15-6 HCAPLUS
CN Sodium bromide (NaBr) (9CI) (CA INDEX NAME)

Br--Na

RN 7681-11-0 HCAPLUS
 CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I-K

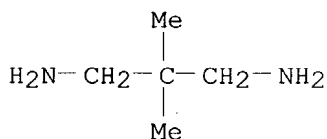
RN 7681-82-5 HCAPLUS
 CN Sodium iodide (NaI) (9CI) (CA INDEX NAME)

I-Na

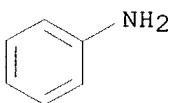
IT 10377-51-2, Lithium iodide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (metalloporphyrin catalysts promoted with, for oxidative carbonylation
 of amines with carbon monoxide in presence of alc.)
 RN 10377-51-2 HCAPLUS
 CN Lithium iodide (LiI) (9CI) (CA INDEX NAME)

I-Li

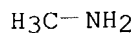
IT 7328-91-8, 2,2-Dimethyl-1,3-propanediamine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative carbonylation of, di-Et isophorone dicarbamate by)
 RN 7328-91-8 HCAPLUS
 CN 1,3-Propanediamine, 2,2-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



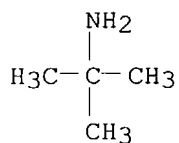
IT 62-53-3, Aniline, reactions 74-89-5, Methylamine,
 reactions 75-64-9, tert-Butylamine, reactions 80-52-4,
 1,8-Diamino-p-menthane 102-07-8 108-44-1, m-Toluidine,
 reactions 108-91-8, Cyclohexylamine, reactions 124-09-4
 , 1,6-Hexanediamine, reactions 1792-17-2 2387-23-7
 2579-20-6, 1,3-Cyclohexanedimethanamine 2855-13-2
 6291-85-6 9046-10-0, Jeffamine D-230
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative carbonylation of, with carbon monoxide in presence of alc.,
 catalytic)
 RN 62-53-3 HCAPLUS
 CN Benzenamine (9CI) (CA INDEX NAME)



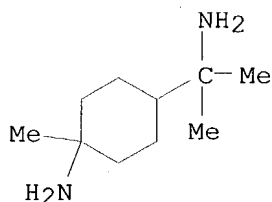
RN 74-89-5 HCAPLUS
CN Methanamine (9CI) (CA INDEX NAME)



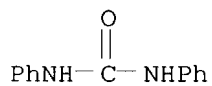
RN 75-64-9 HCAPLUS
CN 2-Propanamine, 2-methyl- (9CI) (CA INDEX NAME)



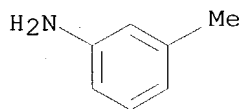
RN 80-52-4 HCAPLUS
CN Cyclohexanemethanamine, 4-amino- α,α ,4-trimethyl- (9CI) (CA INDEX NAME)



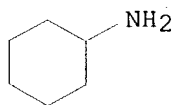
RN 102-07-8 HCAPLUS
CN Urea, N,N'-diphenyl- (9CI) (CA INDEX NAME)



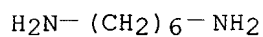
RN 108-44-1 HCAPLUS
CN Benzenamine, 3-methyl- (9CI) (CA INDEX NAME)



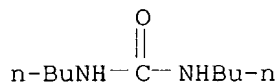
RN 108-91-8 HCAPLUS
CN Cyclohexanamine (9CI) (CA INDEX NAME)



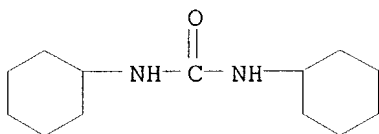
RN 124-09-4 HCAPLUS
CN 1,6-Hexanediamine (7CI, 8CI, 9CI) (CA INDEX NAME)



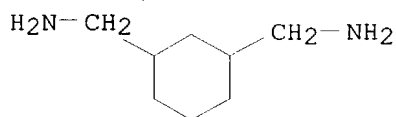
RN 1792-17-2 HCAPLUS
CN Urea, N,N'-dibutyl- (9CI) (CA INDEX NAME)



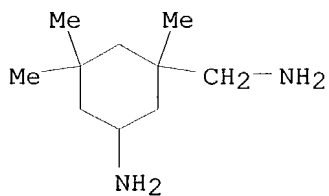
RN 2387-23-7 HCAPLUS
CN Urea, N,N'-dicyclohexyl- (9CI) (CA INDEX NAME)



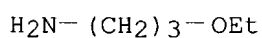
RN 2579-20-6 HCAPLUS
CN 1,3-Cyclohexanedimethanamine (9CI) (CA INDEX NAME)



RN 2855-13-2 HCAPLUS
CN Cyclohexanemethanamine, 5-amino-1,3,3-trimethyl- (9CI) (CA INDEX NAME)

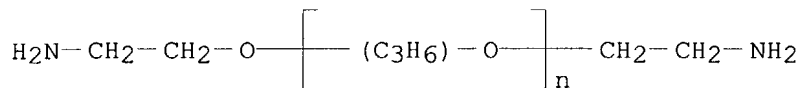


RN 6291-85-6 HCAPLUS
CN 1-Propanamine, 3-ethoxy- (9CI) (CA INDEX NAME)



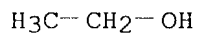
RN 9046-10-0 HCAPLUS
CN Poly[oxy(methyl-1,2-ethanediyl)], α -(2-aminomethylethyl)- ω -(2-

aminomethylethoxy)- (9CI) (CA INDEX NAME)

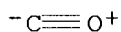


2 (D1-Me)

IT **64-17-5**, Ethanol, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative carbonylation reaction of, with amines and carbon
monoxide, catalytic, carbamates by)
 RN 64-17-5 HCAPLUS
 CN Ethanol (9CI) (CA INDEX NAME)



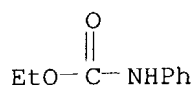
IT **630-08-0**, Carbon monoxide, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative carbonylation with, of amines in presence of alc.,
 carbamates by catalytic)
 RN 630-08-0 HCAPLUS
 CN Carbon monoxide (8CI, 9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, uses
 RL: USES (Uses)
 (oxidizing agent, for oxidative carbonylation of amines with carbon
 monoxide in presence of alc. for carbamate synthesis)
 RN 7782-44-7 HCAPLUS
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)



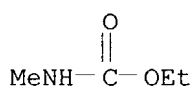
IT **101-99-5P**, Ethyl N-phenylcarbamate **103-69-5P**,
 N-Ethylaniline **105-40-8P**, Ethyl N-methylcarbamate
591-62-8P 1541-19-1P, Ethyl N-cyclohexylcarbamate
1611-50-3P, Ethyl N-t-butylcarbamate **3066-65-7P**
6135-33-7P, Ethyl N-m-tolylcarbamate **83714-43-6P**
86065-40-9P 117658-86-3P 149273-24-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 101-99-5 HCAPLUS
 CN Carbamic acid, phenyl-, ethyl ester (9CI) (CA INDEX NAME)



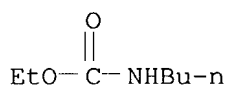
RN 103-69-5 HCAPLUS
CN Benzenamine, N-ethyl- (9CI) (CA INDEX NAME)



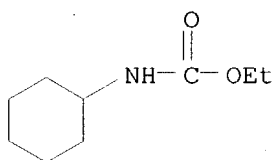
RN 105-40-8 HCAPLUS
CN Carbamic acid, methyl-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



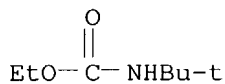
RN 591-62-8 HCAPLUS
CN Carbamic acid, butyl-, ethyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



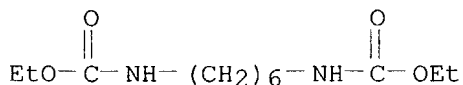
RN 1541-19-1 HCAPLUS
CN Carbamic acid, cyclohexyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 1611-50-3 HCAPLUS
CN Carbamic acid, (1,1-dimethylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

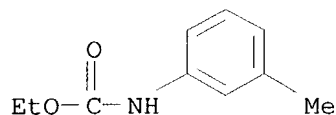


RN 3066-65-7 HCAPLUS
CN Carbamic acid, 1,6-hexanediylbis-, diethyl ester (9CI) (CA INDEX NAME)



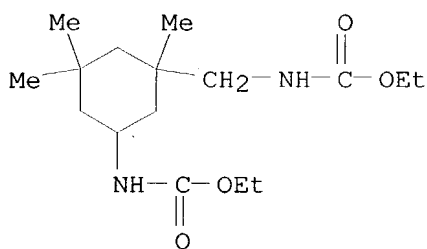
RN 6135-33-7 HCAPLUS

CN Carbamic acid, (3-methylphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



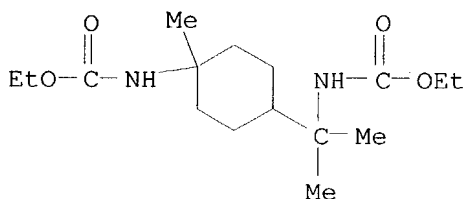
RN 83714-43-6 HCAPLUS

CN Carbamic acid, [3-[[[(ethoxycarbonyl)amino]methyl]-3,5,5-trimethylcyclohexyl]-, ethyl ester (9CI) (CA INDEX NAME)



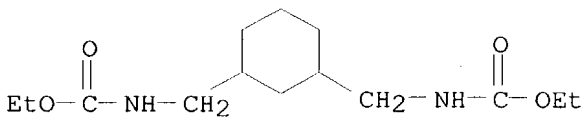
RN 86065-40-9 HCAPLUS

CN Carbamic acid, [1-[4-[(ethoxycarbonyl)amino]-4-methylcyclohexyl]-1-methylethyl]-, ethyl ester (9CI) (CA INDEX NAME)



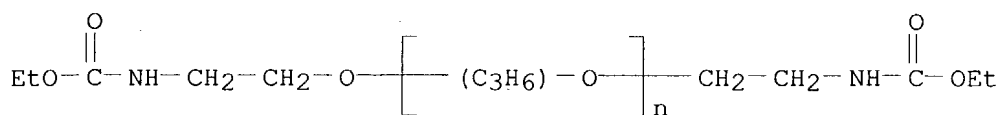
RN 117658-86-3 HCAPLUS

CN Carbamic acid, [1,3-cyclohexanediylbis(methylene)]bis-, diethyl ester (9CI) (CA INDEX NAME)



RN 149273-24-5 HCAPLUS

CN Poly[oxy(methyl-1,2-ethanediyl)], α-[2-[(ethoxycarbonyl)amino]methyl ethyl]-ω-[2-[(ethoxycarbonyl)amino]methylethoxy]- (9CI) (CA INDEX NAME)



2 (D1-Me)

IT 75-13-8DP, Isocyanic acid, esters

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of carbamate reactins for preparation of, via thermal decomposition)

RN 75-13-8 HCAPLUS

CN Isocyanic acid (6CI, 8CI, 9CI) (CA INDEX NAME)

HN=C=O

L43 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:191247 HCAPLUS

DOCUMENT NUMBER: 118:191247

TITLE: Synthesis of cyclohexanol, cyclohexanone, and adipic acid

INVENTOR(S): Liu, Shangchang; Dong, Qiren; et al.

PATENT ASSIGNEE(S): Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|--------------|
| CN 1062718 | A | 19920715 | CN 1992-106038 | 19920129 <-- |
| CN 1048480 | B | 20000119 | | |

PRIORITY APPLN. INFO.: CN 1992-106038 19920129 <--

OTHER SOURCE(S): CASREACT 118:191247

AB The title compds. are prepared by oxidation of cyclohexane (I) over transition metal complexes with electroconducting polymer mol. sieves. This process is simple and fast, it causes no pollution or corrosion, and it increases both yield and selectivity. Pure O (99.95%) was introduced to an autoclave containing I and 10-5-10-7 m/L PdCl₂ complex with polypyrrole in 0.25 mol equivalent (based on I) cyclohexanol or Me₂CO as solvent and the mixture was heated at 140° and 10 atm to give 98% cyclohexanol acid 98% selectivity.

IT 30604-81-0, Polypyrrole

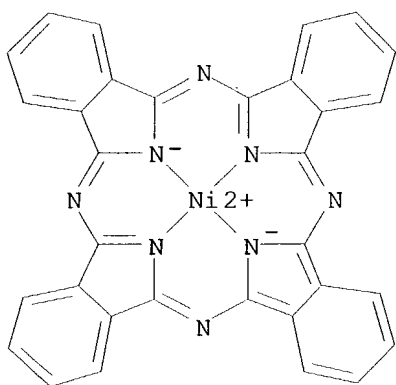
RL: RCT (Reactant); RACT (Reactant or reagent)

(catalysts containing palladium dichloride and, for oxidation of cyclohexane)

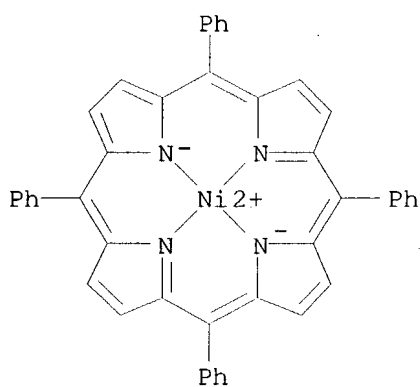
RN 30604-81-0 HCAPLUS

CN 1H-Pyrrole, homopolymer (9CI) (CA INDEX NAME)

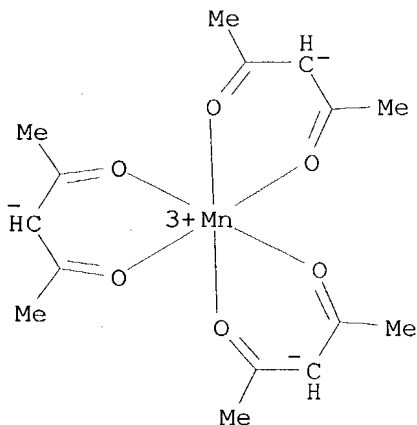
CM 1



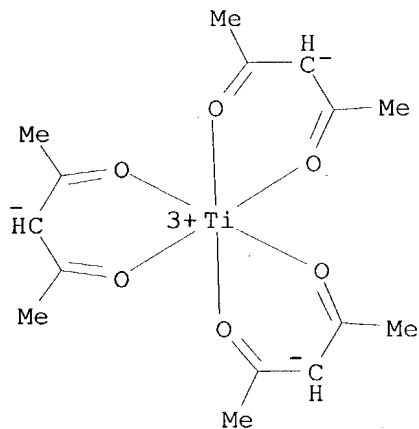
RN 14172-92-0 HCAPLUS
 CN Nickel, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



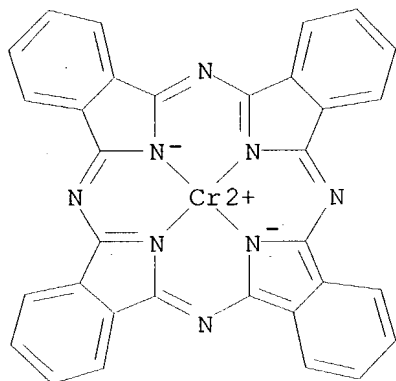
RN 14284-89-0 HCAPLUS
 CN Manganese, tris(2,4-pentanedionato- κ O, κ O')-, (OC-6-11)- (9CI)
 (CA INDEX NAME)



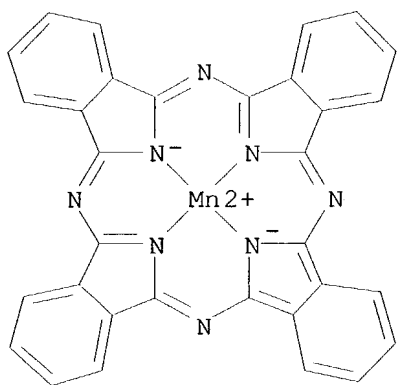
RN 14284-96-9 HCAPLUS
CN Titanium, tris(2,4-pentanedionato- κ O, κ O')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



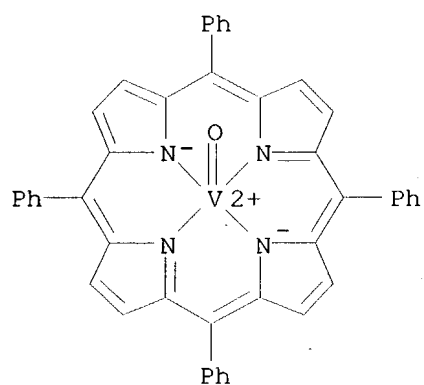
RN 14285-60-0 HCAPLUS
CN Chromium, [29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31,.
 κ N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



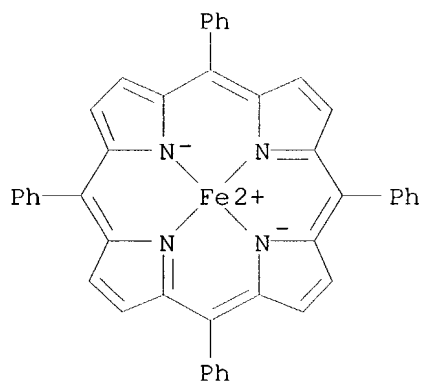
RN 14325-24-7 HCAPLUS
CN Manganese, [29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31,
 κ N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



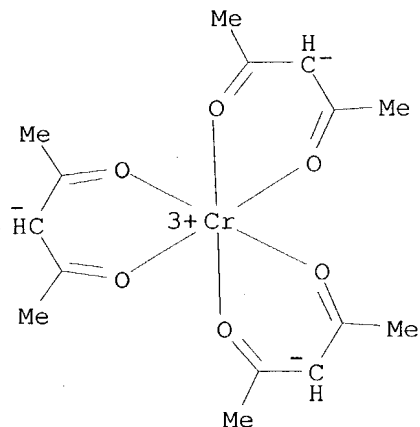
RN 14705-63-6 HCAPLUS
 CN Vanadium, oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-5-12)- (9CI) (CA INDEX
 NAME)



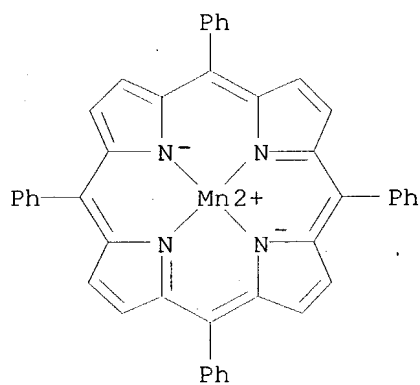
RN 16591-56-3 HCAPLUS
 CN Iron, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



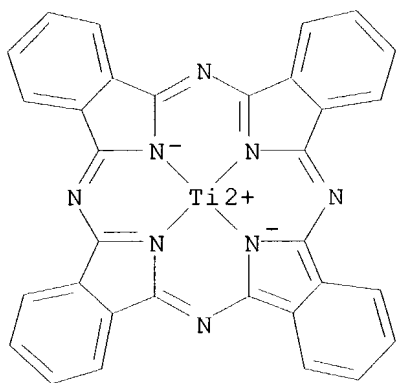
RN 21679-31-2 HCAPLUS
CN Chromium, tris(2,4-pentanedionato- κ O, κ O')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



RN 31004-82-7 HCAPLUS
CN Manganese, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)- κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 52324-93-3 HCAPLUS
CN Titanium, [29H,31H-phthalocyaninato(2-)- κ N29, κ N30, κ N31, κ N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 125491-21-6 HCAPLUS

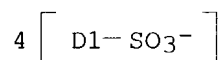
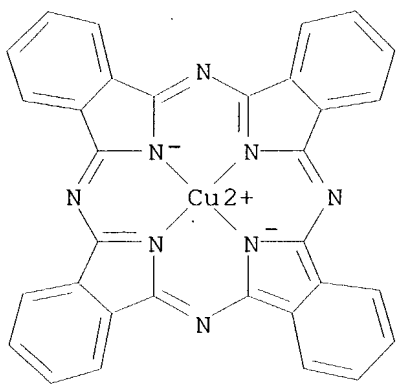
CN Ethanaminium, N,N,N-triethyl-, [29H,31H-phthalocyanine-C,C,C,C-tetrasulfonato(6-)-N29,N30,N31,N32]cuprate(4-) (4:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67462-31-1

CMF C32 H12 Cu N8 O12 S4

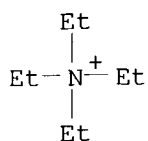
CCI CCS, IDS



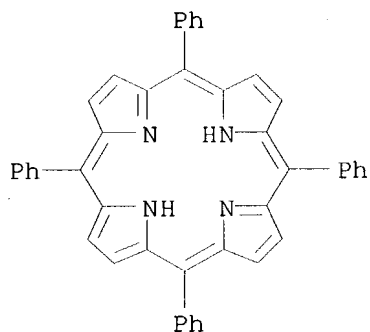
CM 2

CRN 66-40-0

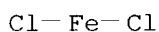
CMF C8 H20 N



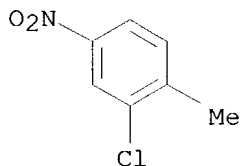
IT **917-23-7**, Tetraphenylporphine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (complexation of, with ferrous chloride)
 RN 917-23-7 HCAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



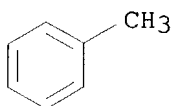
IT **7758-94-3**, Ferrous chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (complexation of, with tetraphenylporphine)
 RN 7758-94-3 HCAPLUS
 CN Iron chloride (FeCl₂) (8CI, 9CI) (CA INDEX NAME)



IT **121-86-8**, 2-Chloro-4-nitrotoluene **61878-61-3**,
 Chloronitrotoluene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, to chloronitrobenzoic acid)
 RN 121-86-8 HCAPLUS
 CN Benzene, 2-chloro-1-methyl-4-nitro- (9CI) (CA INDEX NAME)



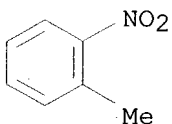
RN 61878-61-3 HCAPLUS
 CN Benzene, methyl-, monochloro mononitro deriv. (9CI) (CA INDEX NAME)



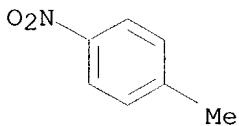
D1-NO₂

D1-Cl

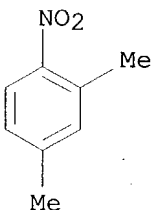
IT **88-72-2, o-Nitrotoluene 99-99-0, p-Nitrotoluene**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, to nitrobenzoic acid)
 RN 88-72-2 HCAPLUS
 CN Benzene, 1-methyl-2-nitro- (9CI) (CA INDEX NAME)



RN 99-99-0 HCAPLUS
 CN Benzene, 1-methyl-4-nitro- (9CI) (CA INDEX NAME)



IT **89-87-2, 4-Nitro-m-xylene 25168-04-1**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, to nitrophthalic acid)
 RN 89-87-2 HCAPLUS
 CN Benzene, 2,4-dimethyl-1-nitro- (9CI) (CA INDEX NAME)



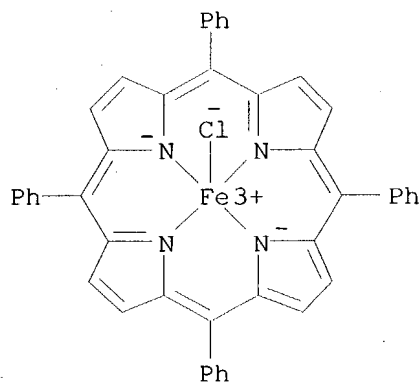
RN 25168-04-1 HCAPLUS
 CN Benzene, dimethylnitro- (9CI) (CA INDEX NAME)



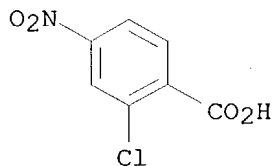
2 (D1-Me)

D1-NO₂

IT **16456-81-8P**, Iron tetraphenylporphine chloride
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as catalysts for oxidation of cyclic hydrocarbons to cyclic
 carboxylic acids)
 RN 16456-81-8 HCAPLUS
 CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX
 NAME)



IT **99-60-5P**, 2-Chloro-4-nitrobenzoic acid **125634-98-2P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidation of chloronitrotoluene)
 RN 99-60-5 HCAPLUS
 CN Benzoic acid, 2-chloro-4-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 125634-98-2 HCAPLUS
 CN Benzoic acid, chloronitro- (9CI) (CA INDEX NAME)

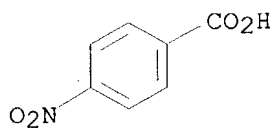


D1-NO₂

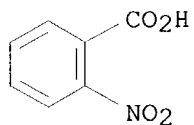
D1-Cl

D1-CO₂H

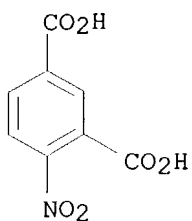
IT 62-23-7P, p-Nitrobenzoic acid 552-16-9P, o-Nitrobenzoic acid
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidation of nitrotoluene)
 RN 62-23-7 HCAPLUS
 CN Benzoic acid, 4-nitro- (9CI) (CA INDEX NAME)



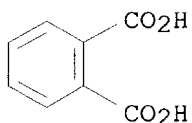
RN 552-16-9 HCAPLUS
 CN Benzoic acid, 2-nitro- (9CI) (CA INDEX NAME)



IT 4315-09-7P, 4-Nitroisophthalic acid 51269-48-8P, Nitrophthalic acid
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidation of nitroxylenes)
 RN 4315-09-7 HCAPLUS
 CN 1,3-Benzenedicarboxylic acid, 4-nitro- (9CI) (CA INDEX NAME)

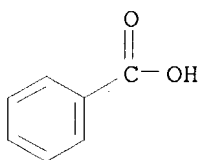


RN 51269-48-8 HCAPLUS
CN 1,2-Benzenedicarboxylic acid, nitro- (9CI) (CA INDEX NAME)

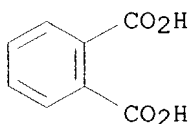


D1-NO2

IT 65-85-0DP, Benzoic acid, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of toluenes)
RN 65-85-0 HCAPLUS
CN Benzoic acid (7CI, 8CI, 9CI) (CA INDEX NAME)



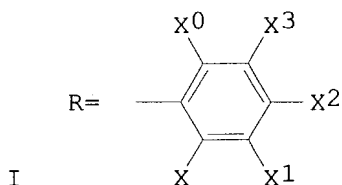
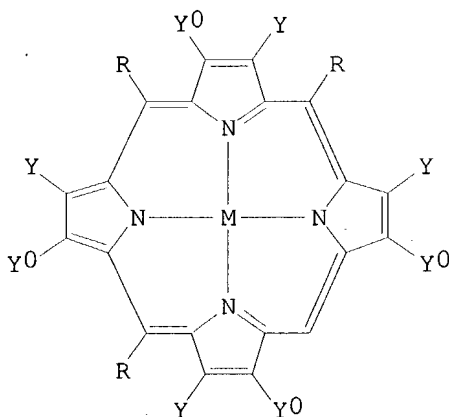
IT 88-99-3DP, 1,2-Benzenedicarboxylic acid, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of xylenes)
RN 88-99-3 HCAPLUS
CN 1,2-Benzenedicarboxylic acid (9CI) (CA INDEX NAME)



L43 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:407144 HCAPLUS
DOCUMENT NUMBER: 111:7144
TITLE: Metalated tetraphenyl porphyrins, their nonmetalated precursors, and their use in the oxidation of lignin,

alkanes, and alkenes
 INVENTOR(S): Dolphin, David H.; Nakano, Taku; Kirk, Thomas Kent;
 Maione, Theodore E.; Farrell, Roberta L.; Wijesekera,
 Tilak Panini
 PATENT ASSIGNEE(S): Can.
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|-----------------|
| WO 8807988 | A1 | 19881020 | WO 1988-US1240 | 19880415 <-- |
| W: AU, DK, FI, JP, KR, NO, SU | | | | |
| RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| AU 8817075 | A1 | 19881104 | AU 1988-17075 | 19880415 <-- |
| AU 617670 | B2 | 19911205 | | |
| US 4892941 | A | 19900109 | US 1988-181859 | 19880415 <-- |
| EP 363379 | A1 | 19900418 | EP 1988-904116 | 19880415 <-- |
| EP 363379 | B1 | 19950614 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| JP 02503086 | T2 | 19900927 | JP 1988-503781 | 19880415 <-- |
| CA 1308096 | A1 | 19920929 | CA 1988-564424 | 19880418 <-- |
| NO 8805571 | A | 19890216 | NO 1988-5571 | 19881215 <-- |
| DK 8807020 | A | 19881216 | DK 1988-7020 | 19881216 <-- |
| KR 9702638 | B1 | 19970307 | KR 1988-71690 | 19881217 <-- |
| FI 92402 | B | 19940729 | FI 1989-4898 | 19891016 <-- |
| FI 92402 | C | 19941110 | | |
| US 5077394 | A | 19911231 | US 1989-455663 | 19891221 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | | US 1987-39566 | A 19870417 <-- |
| | | | US 1988-181859 | A3 19880415 <-- |
| | | | WO 1988-US1240 | A 19880415 <-- |
| OTHER SOURCE(S): MARPAT 111:7144 | | | | |
| GI | | | | |



AB Metalated porphyrins I [M = oxidation-sustaining transition metal, optionally with axial ligand; X, X0 = H, non-H2O-solubilizing electroneg. group;

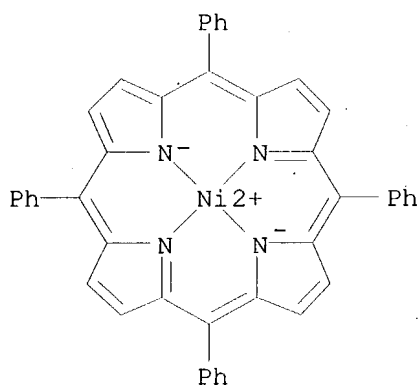
X1-X3 = H, electroneg. group; Y, Y0 = H, F, Cl; Y and/or Y0 \neq H when none of X1-X3 is H2O-soluble; 1-2 of X1-X3 is H2O-soluble and ≥ 2 of X's in non-H2O-soluble electroneg. group when Y = Y0 = H; ≥ 2 of X1-X3 is H2O-soluble] and their salt forms are prepared for use as **oxidation catalysts**, especially for oxidation-degradation of lignin in wood or pulp, hydroxylation of (cyclo)alkanes, and epoxidn. of (cyclo)alkenes. Chloriantion of chloro[meso-tetra-(2,6-dichlorophenyl)porphinato]iron(III) using FeCl3 and Cl at 140° gave 88% of the β -octachloro derivative, which underwent demetalation-sulfonation by fuming H2SO4 at 165° and remetalation by FeCl2.4H2O in DMF to give I (M = Fe with axial Cl ligand, X = X0 = Cl, X1 = X2 = H, X3 = SO3H, Y = Y0 = Cl) (II). Oxidation of 2 g northern softwood kraft by 0.5% (w/v) Me3COOH in buffer at pH 5 and 60° yielded a kappa value of 9.5 in the presence of 90 mg II, vs. 17.6 without II.

IT 14172-92-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(chloriantion of)

RN 14172-92-0 HCAPLUS

CN Nickel, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 $\kappa N21, \kappa N22, \kappa N23, \kappa N24$]-, (SP-4-1)- (9CI) (CA INDEX
NAME)

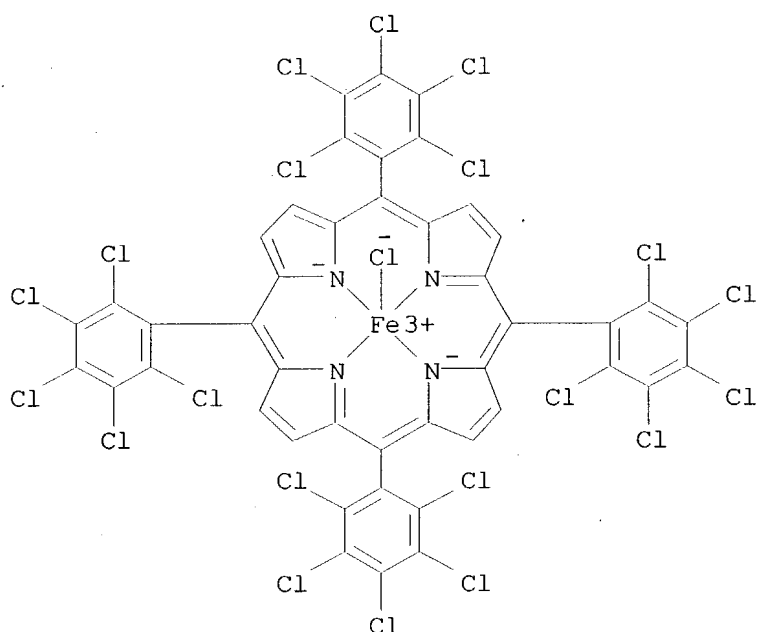


IT 91042-28-3

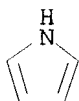
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

RN 91042-28-3 HCAPLUS

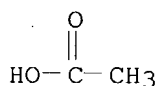
CN Iron, chloro[5,10,15,20-tetrakis(pentachlorophenyl)-21H,23H-porphinato(2-)-
 $\kappa N21, \kappa N22, \kappa N23, \kappa N24$]-, (SP-5-12)- (9CI) (CA INDEX
NAME)



IT 109-97-7, Pyrrole
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with dichlorobenzaldehyde and zinc acetate,
 porphyrin from)
 RN 109-97-7 HCAPLUS
 CN 1H-Pyrrole (9CI) (CA INDEX NAME)



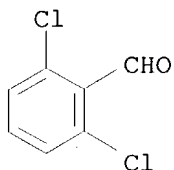
IT 557-34-6, Zinc acetate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with pyrrole and dichlorobenzaldehyde, porphyrin
 from)
 RN 557-34-6 HCAPLUS
 CN Acetic acid, zinc salt (8CI, 9CI) (CA INDEX NAME)



● 1/2 Zn

IT 83-38-5, 2,6-Dichlorobenzaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with pyrrole and zinc acetate, porphyrin from)

RN 83-38-5 HCAPLUS
CN Benzaldehyde, 2,6-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



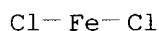
IT 110-83-8, Cyclohexene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(epoxidn. of, using porphyrin catalysts)
RN 110-83-8 HCAPLUS
CN Cyclohexene (8CI, 9CI) (CA INDEX NAME)



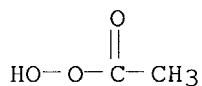
IT 110-82-7, Cyclohexane, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroxylation of, using porphyrin catalysts)
RN 110-82-7 HCAPLUS
CN Cyclohexane (8CI, 9CI) (CA INDEX NAME)



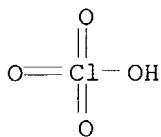
IT 7758-94-3, Ferrous chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(metalation by, of chlorianted porphyrin derivative)
RN 7758-94-3 HCAPLUS
CN Iron chloride (FeCl₂) (8CI, 9CI) (CA INDEX NAME)



IT 79-21-0, Peracetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation by, of lignin, using porphyrin catalysts)
RN 79-21-0 HCAPLUS
CN Ethaneperoxoic acid (9CI) (CA INDEX NAME)



IT 7601-89-0, Sodium perchlorate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation by, of pulp, using porphyrin catalysts)
 RN 7601-89-0 HCAPLUS
 CN Perchloric acid, sodium salt (8CI, 9CI) (CA INDEX NAME)

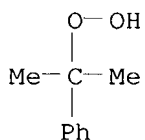


● Na

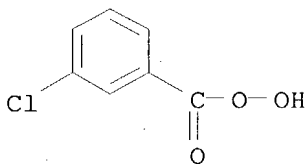
IT 75-91-2, tert-Butyl hydroperoxide 80-15-9, Cumyl hydroperoxide 937-14-4, m-Chloroperbenzoic acid 7681-52-9, Sodium hypochlorite 7722-84-1, Hydrogen peroxide, reactions 7790-21-8 14353-90-3, Pentafluoriodosobenzene 120644-28-2, Iodosoethane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation by, of veratryl alc., using porphyrin catalysts)
 RN 75-91-2 HCAPLUS
 CN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME)

HO-O-Bu-t

RN 80-15-9 HCAPLUS
 CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



RN 937-14-4 HCAPLUS
 CN Benzenecarboperoxoic acid, 3-chloro- (9CI) (CA INDEX NAME)



RN 7681-52-9 HCAPLUS
 CN Hypochlorous acid, sodium salt (8CI, 9CI) (CA INDEX NAME)

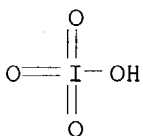


● Na

RN 7722-84-1 HCAPLUS
CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

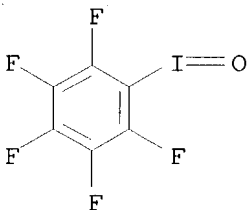


RN 7790-21-8 HCAPLUS
CN Periodic acid (HIO₄), potassium salt (8CI, 9CI) (CA INDEX NAME)

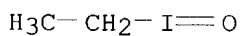


● K

RN 14353-90-3 HCAPLUS
CN Benzene, pentafluoriodosyl- (9CI) (CA INDEX NAME)



RN 120644-28-2 HCAPLUS
CN Ethane, iodosyl- (9CI) (CA INDEX NAME)

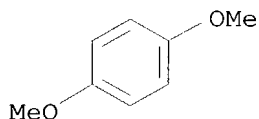


IT 8068-05-1, Indulin AT
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, by peracetic acid using porphyrin catalysts)
RN 8068-05-1 HCAPLUS
CN Lignin, alkali (9CI) (CA INDEX NAME)

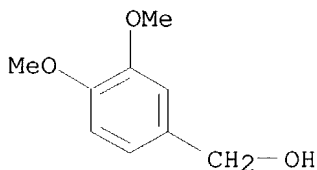
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 150-78-7, 1,4-Dimethoxybenzene
RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of, by tert-Bu peroxide, with porphyrin catalysts)
 RN 150-78-7 HCAPLUS
 CN Benzene, 1,4-dimethoxy- (9CI) (CA INDEX NAME)



IT 93-03-8, Veratryl alcohol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, using porphyrin catalysts)
 RN 93-03-8 HCAPLUS
 CN Benzenemethanol, 3,4-dimethoxy- (9CI) (CA INDEX NAME)



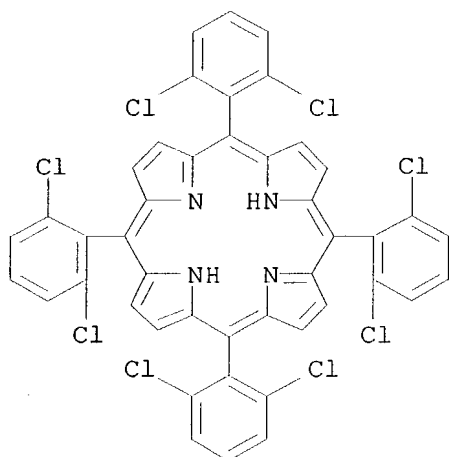
IT 42613-30-9, Ligninase
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation with porphyrin catalysts in comparison to)
 RN 42613-30-9 HCAPLUS
 CN Ligninase (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 9005-53-2, Lignin, reactions
 RL: PRP (Properties)
 (oxidation-degradation of, porphyrin catalysts for)
 RN 9005-53-2 HCAPLUS
 CN Lignin (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 120644-23-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and UV-visible spectrum of)
 RN 120644-23-7 HCAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,6-dichlorophenyl)-, conjugate diacid (9CI) (CA INDEX NAME)



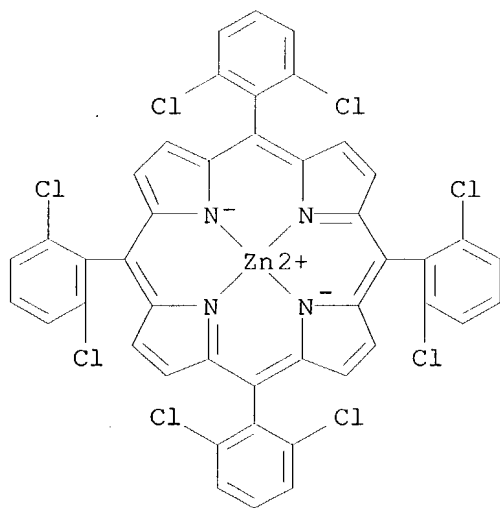
● 2 H⁺

IT 100506-72-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demetalation of)

RN 100506-72-7 HCAPLUS

CN Zinc, [5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



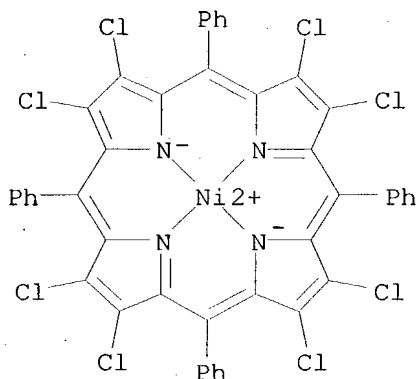
IT 120659-44-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and demetalation or sulfonation-demetalation of)

RN 120659-44-1 HCAPLUS

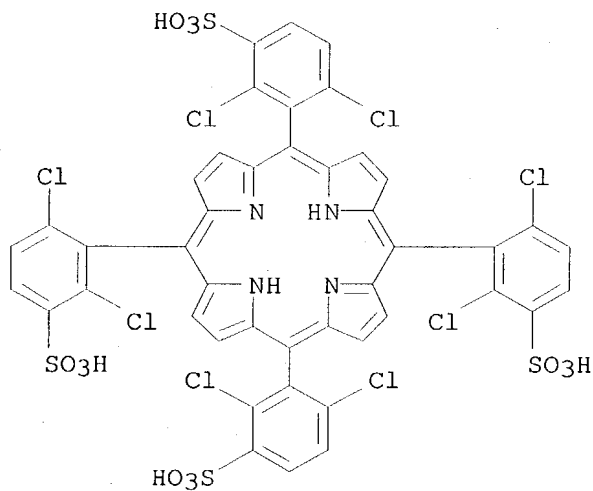
CN Nickel, [2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)-

(9CI) (CA INDEX NAME)


IT 120644-24-8P 120644-25-9P 120644-26-0P
120644-27-1P

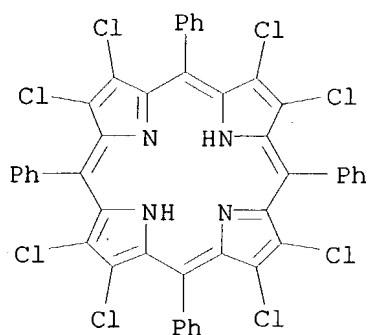
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and metalation of)

RN 120644-24-8 HCAPLUS

CN Benzenesulfonic acid, 3,3',3'',3'''-(21H,23H-porphine-5,10,15,20-
tetrayl)tetrakis[2,4-dichloro- (9CI) (CA INDEX NAME)


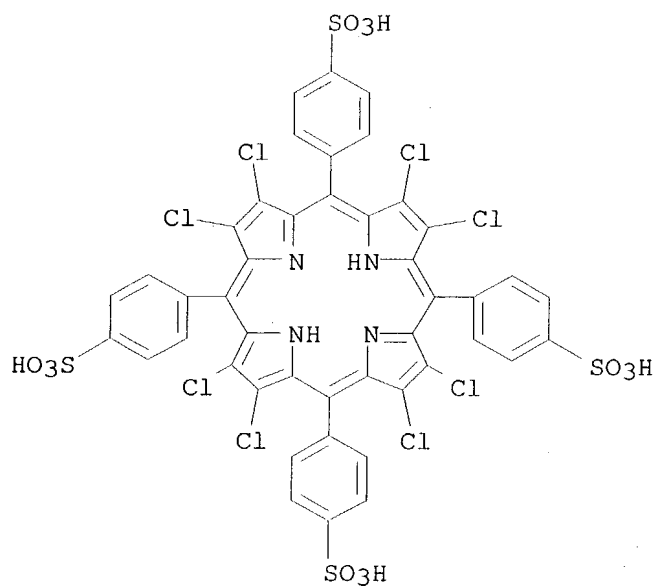
RN 120644-25-9 HCAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)



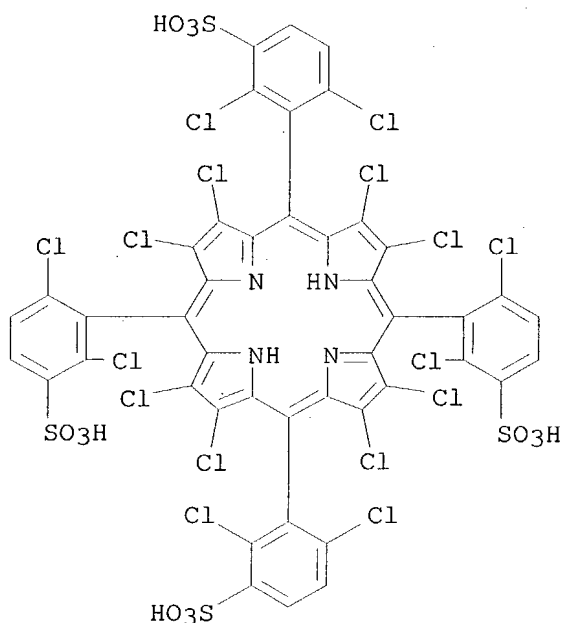
RN 120644-26-0 HCAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)



RN 120644-27-1 HCAPLUS

CN Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[2,4-dichloro- (9CI) (CA INDEX NAME)

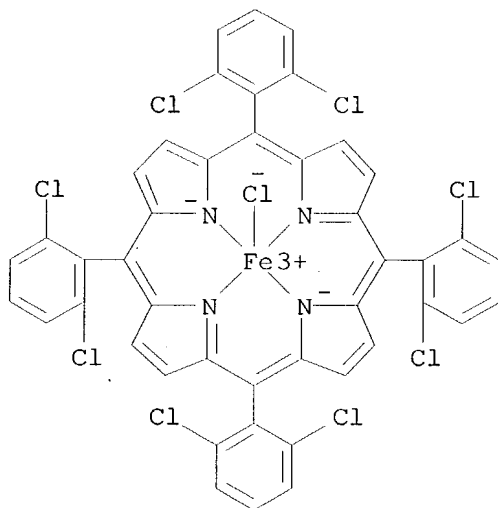


IT 91042-27-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 91042-27-2 HCAPLUS

CN Iron, chloro[5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA
INDEX NAME)



IT 120659-41-8P 120659-42-9P 120659-43-0P

120676-09-7P 120676-10-0P 120676-11-1P

120751-65-7P 120751-66-8P 120751-67-9P

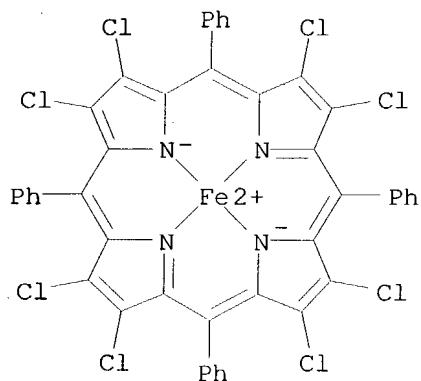
120751-68-0P 120772-68-1P 120772-69-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as **oxidation catalyst** for lignin and

hydrocarbons)

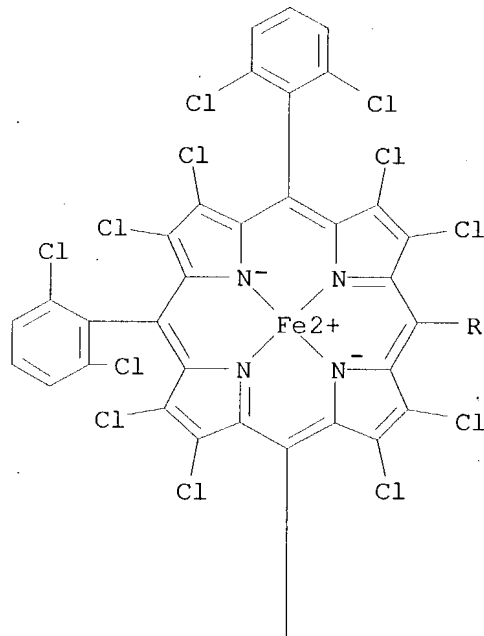
RN 120659-41-8 HCAPLUS

CN Iron, [2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



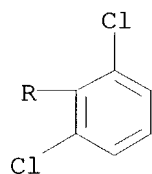
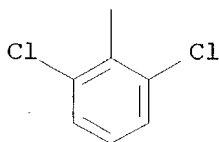
RN 120659-42-9 HCAPLUS

CN Iron, [2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



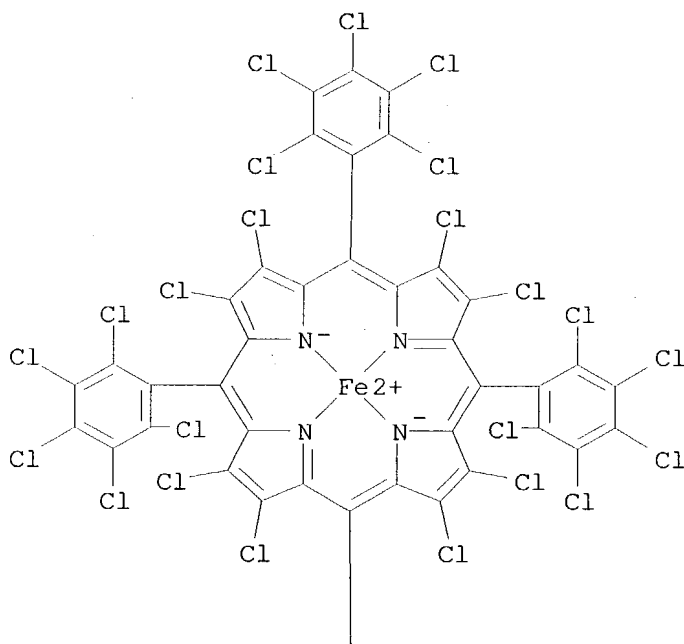
PAGE 1-A

PAGE 2-A

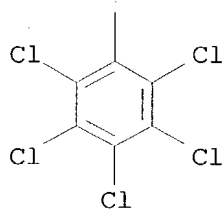


RN 120659-43-0 HCAPLUS
 CN Iron, [2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentachlorophenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-4-1)- (9Cl) (CA INDEX NAME)

PAGE 1-A

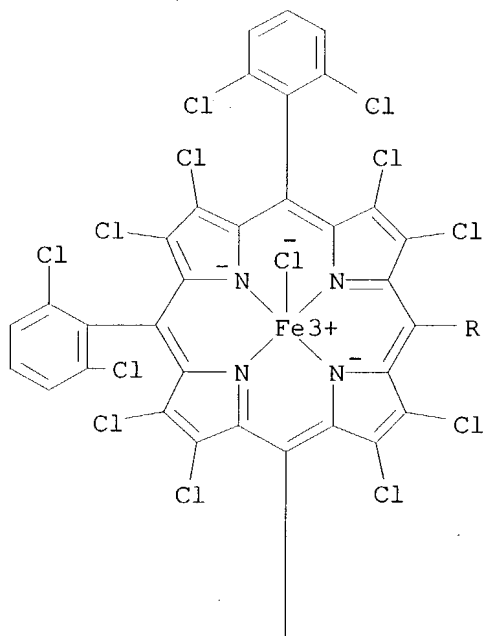


PAGE 2-A

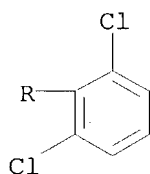
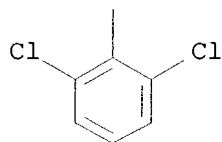


RN 120676-09-7 HCAPLUS
 CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

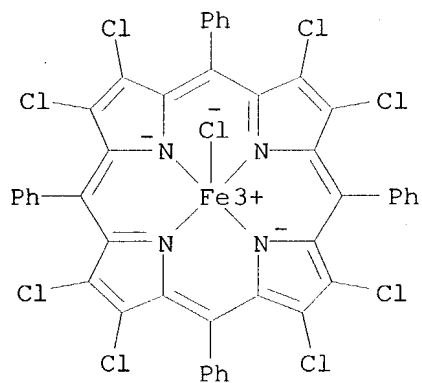
PAGE 1-A



PAGE 2-A

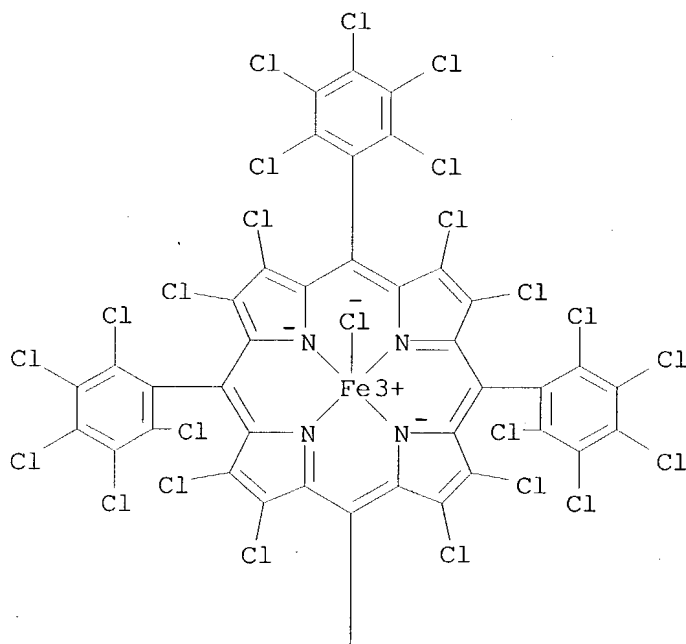


RN 120676-10-0 HCAPLUS
 CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

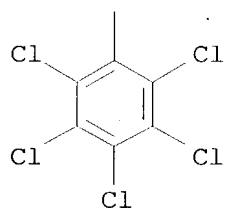


RN 120676-11-1 HCAPLUS
 CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentachlorophenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

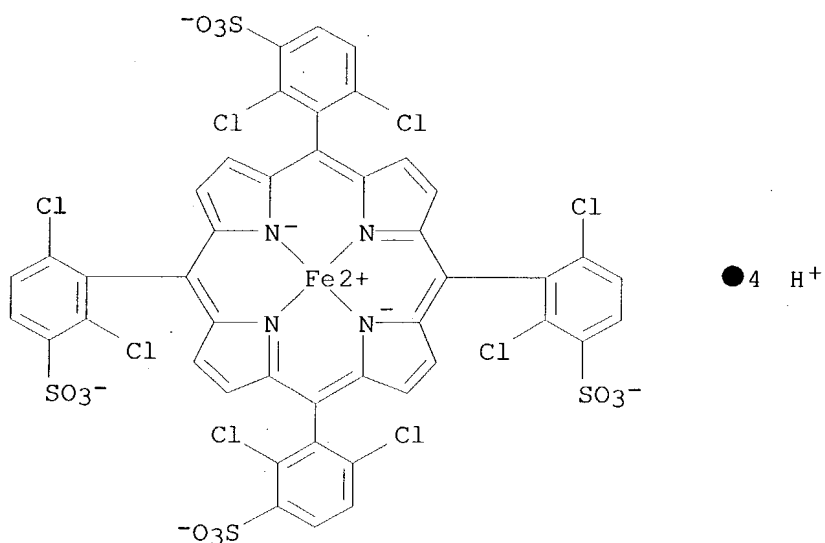
PAGE 1-A



PAGE 2-A

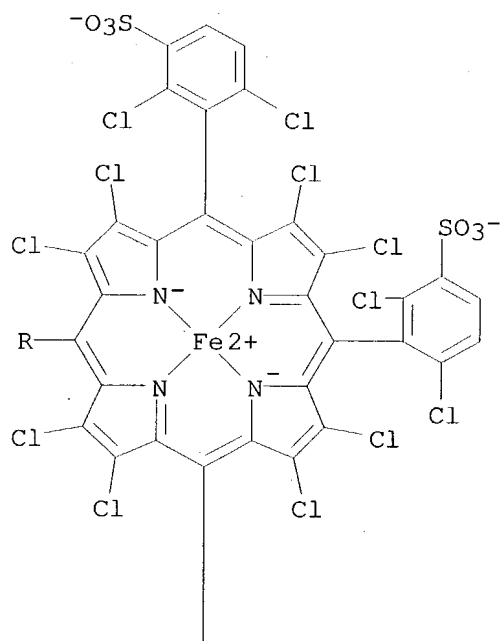


RN 120751-65-7 HCAPLUS
 CN Ferrate(4-), [[3,3',3'',3'''-(21H,23H-porphine-5,10,15,20-tetrayl-
 κN21,κN22,κN23,κN24)tetrakis[2,4-
 dichlorobenzenesulfonato]](6-)]-, tetrahydrogen, (SP-4-1)- (9CI) (CA
 INDEX NAME)

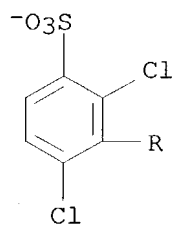
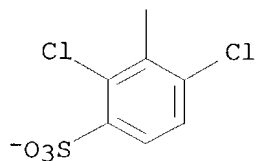


RN 120751-66-8 HCAPLUS
 CN Ferrate(4-), [[{3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl-κN21,κN22,κN23,κN24)te
 trakis[2,4-dichlorobenzenesulfonato]](6-)]-, tetrahydrogen, (SP-4-1)-
 (9CI) (CA INDEX NAME)

PAGE 1-A



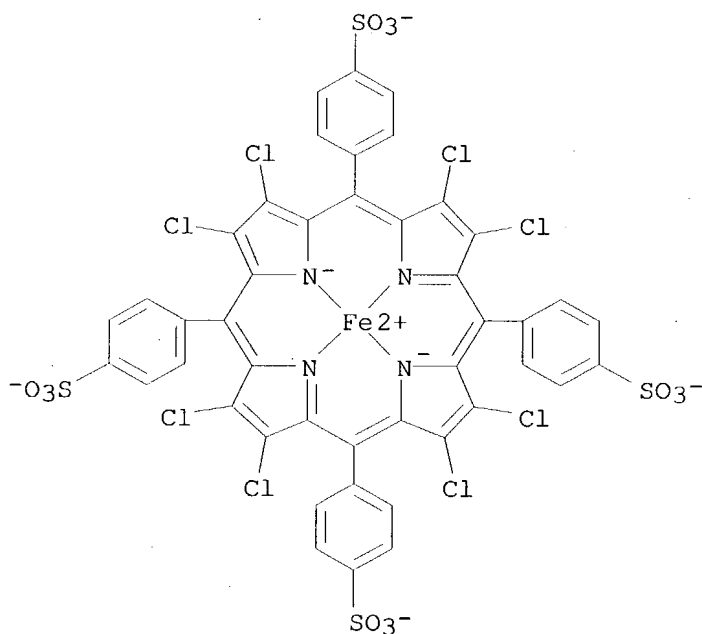
PAGE 2-A



● 4 H⁺

RN 120751-67-9 HCAPLUS
 CN Ferrate(4-), [[4,4',4'',4'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[benzenesulfonato]](6-)-N21,N22,N23,N24]-, tetrahydrogen, (SP-4-1)-(9CI) (CA INDEX NAME)

PAGE 1-A

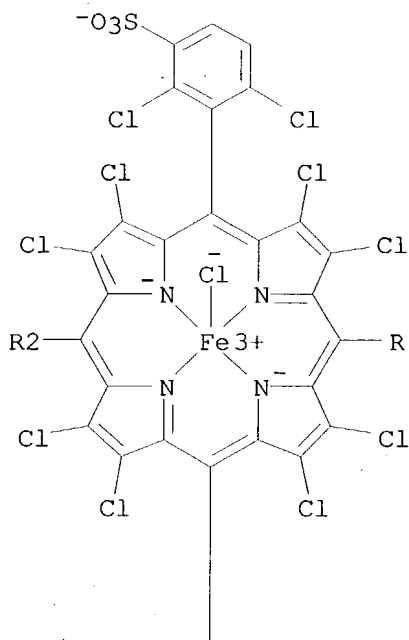


PAGE 2-A

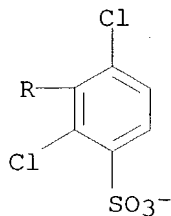
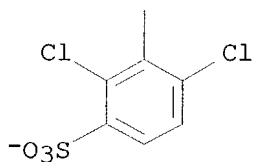
● 4 H⁺

RN 120751-68-0 HCAPLUS
 CN Ferrate(4-), chloro[[3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[2,4-dichlorobenzenesulfonato]](6-)-N21,N22,N23,N24]-, tetrahydrogen, (SP-5-12)-(9CI) (CA INDEX NAME)

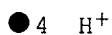
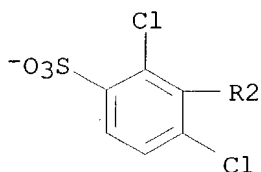
PAGE 1-A



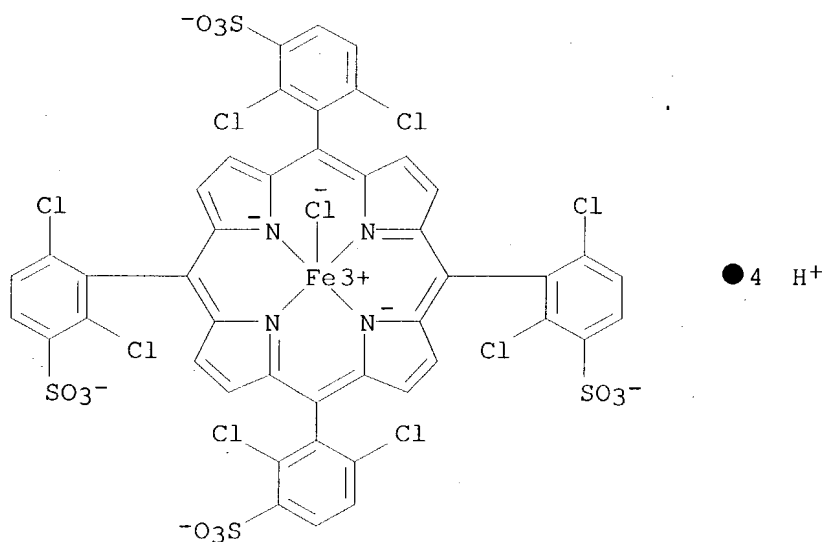
PAGE 2-A



PAGE 3-A

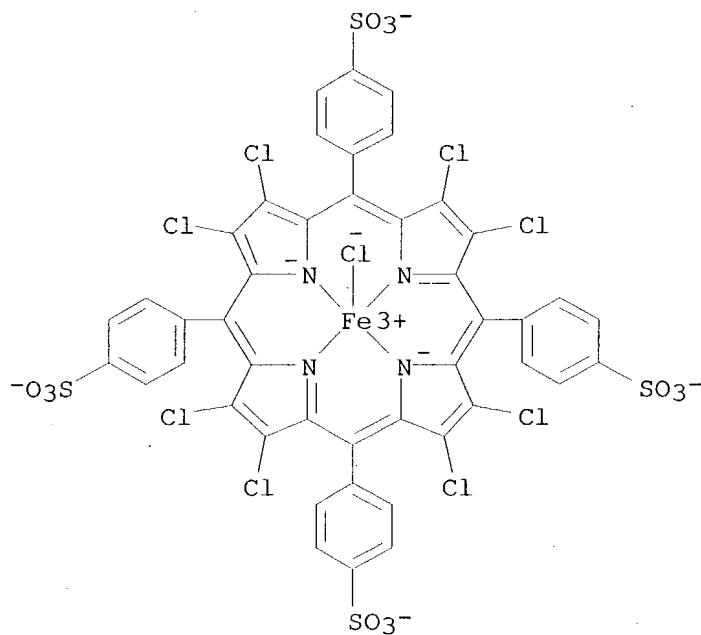


RN 120772-68-1 HCAPLUS
 CN Ferrate(4-), chloro[[3,3',3'',3'''-(21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[2,4-dichlorobenzenesulfonato]](6-)-N21,N22,N23,N24]-, tetrahydrogen, (SP-5-12)- (9CI) (CA INDEX NAME)



RN 120772-69-2 HCAPLUS
 CN Ferrate(4-), chloro[[4,4',4'',4'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[benzenesulfonato]](6-)-N21,N22,N23,N24]-, tetrahydrogen, (SP-5-12)- (9CI) (CA INDEX NAME)

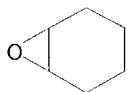
PAGE 1-A



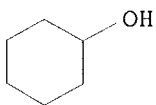
PAGE 2-A

● 4 H⁺

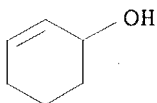
IT **286-20-4P**, Cyclohexene oxide
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by epoxidn. of cyclohexene using porphyrin catalysts)
 RN 286-20-4 HCAPLUS
 CN 7-Oxabicyclo[4.1.0]heptane (8CI, 9CI) (CA INDEX NAME)



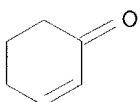
IT **108-93-0P**, Cyclohexanol, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by hydroxylation of cyclohexane, using porphyrin catalysts)
 RN 108-93-0 HCAPLUS
 CN Cyclohexanol (8CI, 9CI) (CA INDEX NAME)



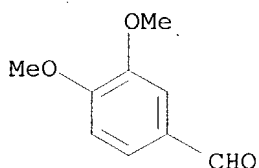
IT 822-67-3P, Cyclohex-2-en-1-ol 930-68-7P,
Cyclohex-2-en-1-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of cyclohexene using porphyrin catalysts)
RN 822-67-3 HCAPLUS
CN 2-Cyclohexen-1-ol (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 120-14-9P, Veratrylaldehyde
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of veratryl alc. using porphyrin catalysts)
RN 120-14-9 HCAPLUS
CN Benzaldehyde, 3,4-dimethoxy- (9CI) (CA INDEX NAME)



IT 9004-34-6 9005-53-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(pulp, degradation of lignin in, porphyrins as catalysts for)
RN 9004-34-6 HCAPLUS
CN Cellulose (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 9005-53-2 HCAPLUS
CN Lignin (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 9004-34-6 9005-53-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(pulp, thermomech., degradation of lignin in, porphyrins as catalysts for)
RN 9004-34-6 HCAPLUS
CN Cellulose (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 9005-53-2 HCAPLUS
CN Lignin (8CI, 9CI) (CA INDEX NAME)

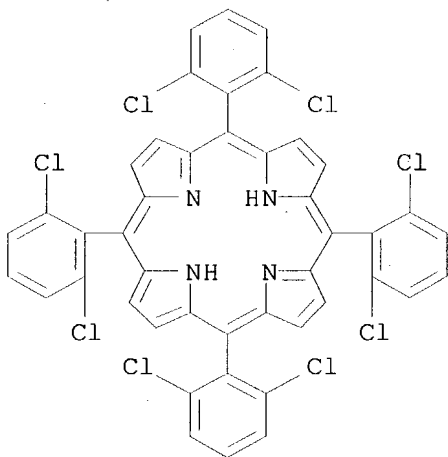
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 37083-37-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfonation and metalation of)

RN 37083-37-7 HCAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA
INDEX NAME)



L43 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:226727 HCAPLUS

DOCUMENT NUMBER: 102:226727

TITLE: Hydrated titanium oxide loaded with
cobalt-tetraphenyl-porphine as **oxidation**
catalyst for carbon monoxide and hydrogen

PATENT ASSIGNEE(S): Titan Kogyo K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|--------------|
| JP 60031827 | A2 | 19850218 | JP 1983-140498 | 19830802 <-- |
| JP 04011258 | B4 | 19920227 | | |

PRIORITY APPLN. INFO.: JP 1983-140498 19830802 <--

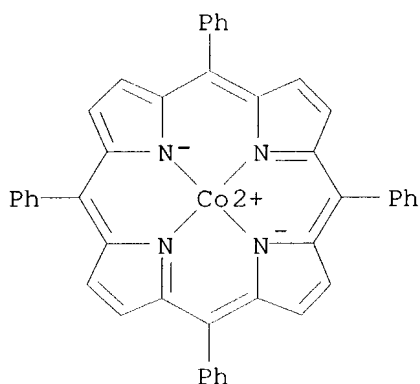
AB Metatitanic acid is dried at $\leq 300^\circ$, the hydrated TiO_2 of sp.
surface area $\geq 170 \text{ m}^2/\text{g}$ is loaded with 1-30% Co-
tetraphenylporphine(I), optionally further evacuated at $150\text{--}350^\circ$,
and is used for oxidation of CO and H_2 with NO and of CO with O_2 . Thus,
metatitanic acid from aqueous TiOSO_4 hydrolysis was washed, dried at
 120° , 10 g $\text{TiO}_2 \cdot x\text{H}_2\text{O}$ ($241.7 \text{ m}^2/\text{g}$) was stirred in 500 mL C_6H_6 containing
0.5 g I overnight, evaporated to dryness to be loaded with 5% I, and evacuated
at 250° for 2 h. A 800 mL mixture of NO 10 and CO 20 torr; CO 5 and
 O_2 10; or NO 2 and H_2 20 was circulated over the 4 g catalyst at 500
mL/min and 100° , $0\text{--}17^\circ$, or 100° , resp. The NO reduction,
CO oxidation after 15 min each, and NO reduction after 45 min were all 100%.

IT 14172-90-8

RL: CAT (Catalyst use); USES (Uses)

(catalyst, on titania support, for oxidation of carbon monoxide and hydrogen)

RN 14172-90-8 HCAPLUS

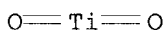
CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

IT 13463-67-7, uses and miscellaneous

RL: CAT (Catalyst use); USES (Uses)

(catalyst, with cobalt tetraphenylporphine for oxidation of carbon monoxide and hydrogen)

RN 13463-67-7 HCAPLUS

CN Titanium oxide (TiO₂) (8CI, 9CI) (CA INDEX NAME)

IT 10102-43-9, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation by, of carbon monoxide and hydrogen on cobalt tetraphenylporphine complex-titania catalyst)

RN 10102-43-9 HCAPLUS

CN Nitrogen oxide (NO) (8CI, 9CI) (CA INDEX NAME)



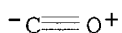
IT 630-08-0, reactions 1333-74-0, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of, on cobalt tetraphenylporphine-titania catalyst)

RN 630-08-0 HCAPLUS

CN Carbon monoxide (8CI, 9CI) (CA INDEX NAME)



RN 1333-74-0 HCAPLUS

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

L43 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

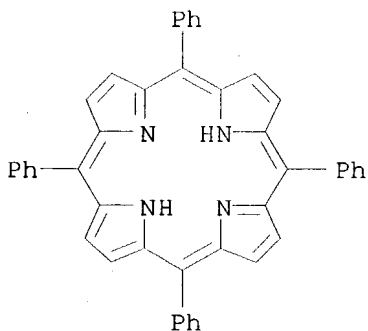
ACCESSION NUMBER: 1981:65319 HCAPLUS
 DOCUMENT NUMBER: 94:65319
 TITLE: Hydroperoxides
 INVENTOR(S): Coltrin, Michael E.; Wu, Yulin
 PATENT ASSIGNEE(S): Phillips Petroleum Co., USA
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| US 4202992 | A | 19800513 | US 1978-883018 | 19780303 <-- |
| US 4269734 | A | 19810526 | US 1980-114923 | 19800124 <-- |
| PRIORITY APPLN. INFO.: | | | US 1978-883018 | 19780303 <-- |

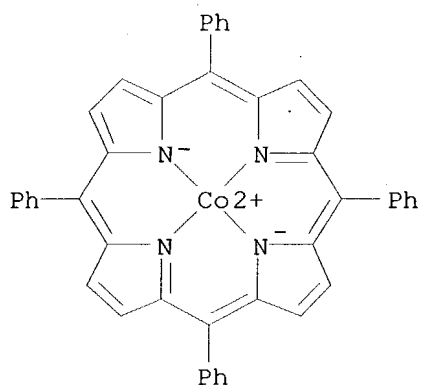
AB Cyclohexylbenzene hydroperoxide (I) was prepared by oxidation of cyclohexylbenzene with O in the absence of light and in the presence of a Cu or a Ni porphine complex. In a typical run, oxidation at 120° for 1.5 h with 200-225 psig initial O pressure using $\alpha,\beta,\gamma,\delta$ -tetraphenylporphinatonicel as a catalyst and I as an initiator gave 80.7 mol% selectivity to I and 13.6 mol% conversion.

IT 917-23-7 14172-90-8 14172-91-9
 14172-92-0 22112-86-3 25482-27-3
 41699-93-8 75279-20-8 75286-28-1
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, for oxidation of cyclohexylbenzenes to hydroperoxide)

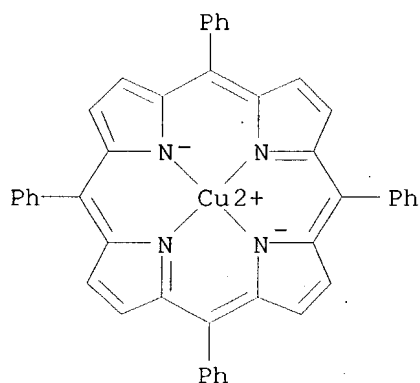
RN 917-23-7 HCAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



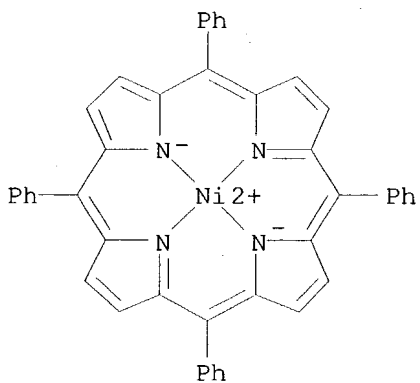
RN 14172-90-8 HCAPLUS
 CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 $\kappa N21,\kappa N22,\kappa N23,\kappa N24$]-, (SP-4-1)- (9CI) (CA INDEX NAME)



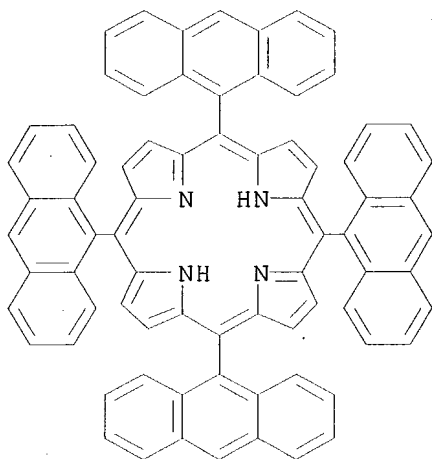
RN 14172-91-9 HCAPLUS
 CN Copper, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



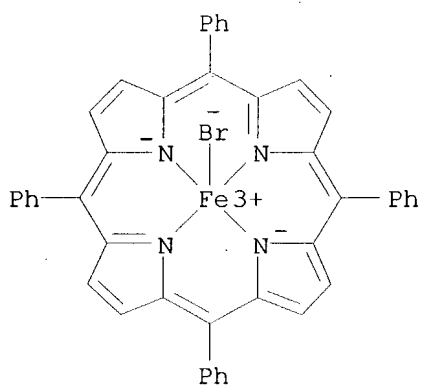
RN 14172-92-0 HCAPLUS
 CN Nickel, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



RN 22112-86-3 HCAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetra-9-anthracenyl- (9CI) (CA INDEX NAME)

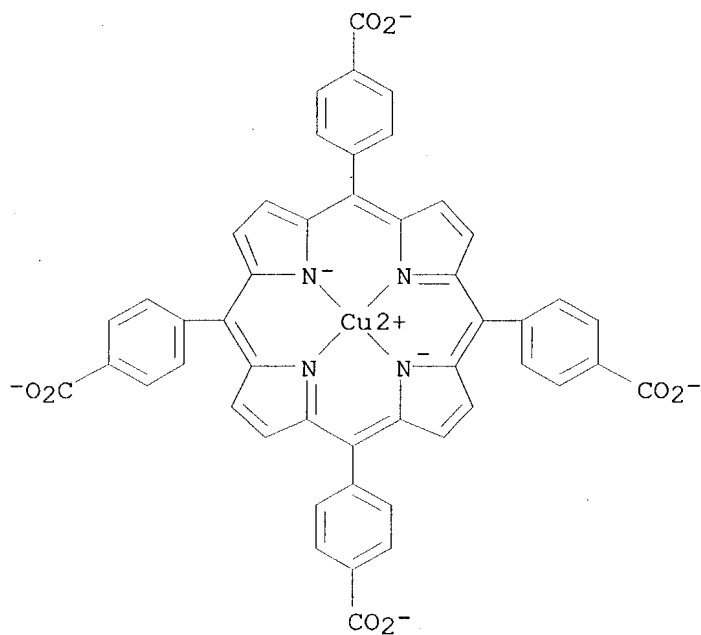


RN 25482-27-3 HCAPLUS
CN Iron, bromo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



RN 41699-93-8 HCAPLUS
CN Cuprate(4-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-
 κ N21, κ N22, κ N23, κ N24)tetrakis[benzoato]](6-)]-,
tetrahydrogen, (SP-4-1)- (9CI) (CA INDEX NAME)

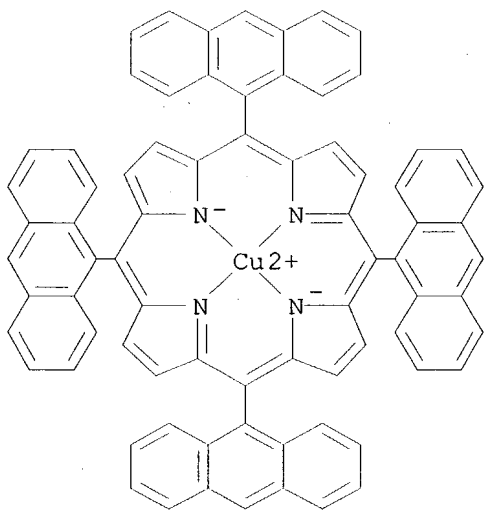
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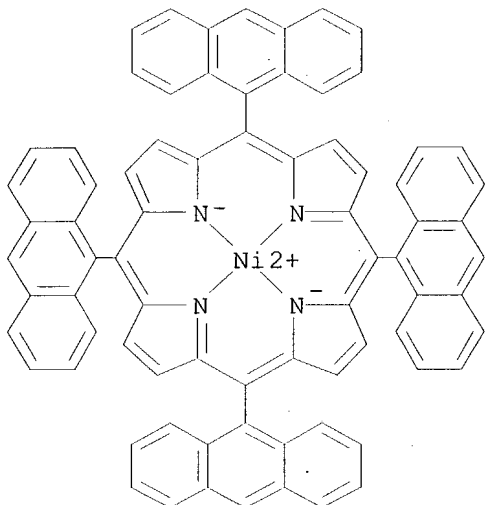
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● 4 H^+

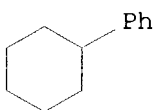
RN 75279-20-8 HCAPLUS
 CN Copper, [5,10,15,20-tetra-9-anthracenyl-21H,23H-porphinato(2-)-
 N21,N22,N23,N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



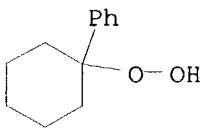
RN 75286-28-1 HCAPLUS
 CN Nickel, [5,10,15,20-tetra-9-anthracenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT 827-52-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, hydroperoxide from, catalyst for)
 RN 827-52-1 HCAPLUS
 CN Benzene, cyclohexyl- (8CI, 9CI) (CA INDEX NAME)



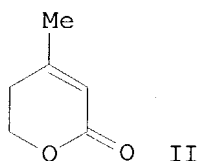
IT 20614-61-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by oxidation of cyclohexylbenzene, catalyst for)
 RN 20614-61-3 HCAPLUS
 CN Hydroperoxide, 1-phenylcyclohexyl (6CI, 8CI, 9CI) (CA INDEX NAME)



L43 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1976:164608 HCAPLUS
 DOCUMENT NUMBER: 84:164608
 TITLE: 3-Methyl-2,4-pentadien-1-al and/or
 4-methyl-5,6-dihydro- α -pyron
 INVENTOR(S): Oka, Masaya; Fujiwara, Yuzuru; Itoi, Kazuo
 PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------------|------|----------|-----------------|--------------|
| JP 50151810 | A2 | 19751206 | JP 1974-60640 | 19740529 <-- |
| JP 60021987 | B4 | 19850530 | | |
| PRIORITY APPLN. INFO.: GI | | | JP 1974-60640 | 19740529 <-- |



AB CH₂:CHCMe:CHCHO (I) and(or) 4-methyl-5,6-dihydro- α -pyrone (II) were prepared by liquid phase reaction of 4-methyl-5,6-dihydro- α -pyran (III) with mol. O in the presence of transition metal salts or complexes. Thus, 0.7-1.0 l./min O was introduced into a mixture of 294 g III and 1 g tetraphenylporphyrin Co complex 90 min at 2-35° to give 82 g unreacted III, 75 g I, and 125 g II.

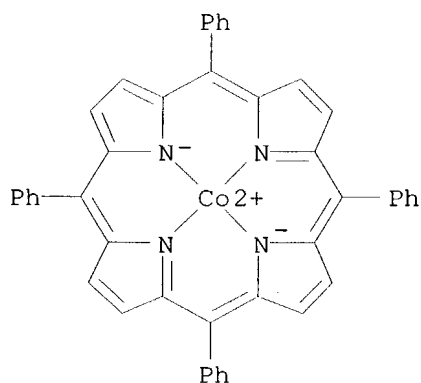
IT 14172-90-8

RL: CAT (Catalyst use); USES (Uses)

(oxidation catalyst, for dihydropyrans with oxygen)

RN 14172-90-8 HCAPLUS

CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)- κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

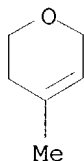


IT 16302-35-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of)

RN 16302-35-5 HCAPLUS

CN 2H-Pyran, 3,6-dihydro-4-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

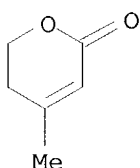


IT 2381-87-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2381-87-5 HCAPLUS

CN 2H-Pyran-2-one, 5,6-dihydro-4-methyl- (8CI, 9CI) (CA INDEX NAME)



L43 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:547298 HCAPLUS

DOCUMENT NUMBER: 83:147298

TITLE: Isopropylbenzene hydroperoxides

INVENTOR(S): Oka, Masanari; Nakamura, Michihiro; Fujisawa, Yuzuru

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| JP 50037741 | A2 | 19750408 | JP 1973-91191 | 19730813 <-- |
| PRIORITY APPLN. INFO.: | | | JP 1973-91191 | 19730813 <-- |

GI For diagram(s), see printed CA Issue.

AB Peroxides (I; R = alkyl except iso-Pr, OH, alkoxy, or halo; $l \geq 0$, $m \geq 1$, $l + m \leq 6$, $1 \leq n \leq m$), useful as oxidizing

agents or polymerization initiators, were prepared by oxidation of the corresponding

benzene derivs., $RlC_6H_6-(l+m)(CHMe_2)_m$, with mol. O in the presence of an organic Co complex in which Co is coordinated with ≥ 4 N atoms. Thus, to a stirring mixture of 10.0 g cumene and 0.01 g tetraphenylporphyrin Co complex (II) was fed O at 70° for 240 min to give 30.7% PhCMe₂OOH, 1.69% PhCMe₂OH, and 0.11% AcPh. Similar results were obtained with Co complexes of tetra(p-methylphenyl)porphyrin, tetra(p-methoxyphenyl)porphyrin, dimethylglyoximepyridine, phthalocyanine, and o-aminobenzaldehyde ethylenediimine. 4-Isopropylphenol gave 10.15% p-HOC₆H₄CMe₂OOH in 10 hrs using 0.01 g II. P-C₆H₄(CHMe₂) (10.0 g) gave 4-Me₂CHC₆H₄CMe₂OOH and p-C₆H₄(CMe₂OOH)₂ at 2:1 ratio at 65° for 7 hr using 0.13 g II (74.69% conversion). Oxidation of p-MeC₆H₄CHMe₂ (10 g) in the presence of 0.007 g II and NaOH (0.025 g of 20.0 weight% solution) at

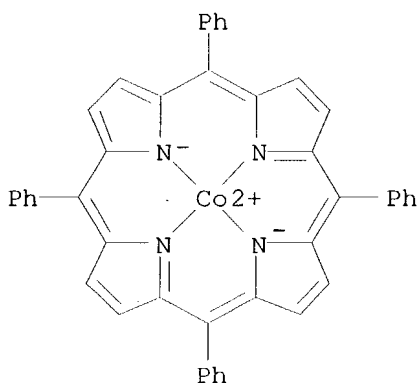
65° for 5 hrs gave 43.92% p-MeC₆H₄CMe₂OOH, 3.31% p-MeC₆H₄CMe₂OH, and 0.61% p-MeC₆H₄Ac. Addition of a peroxide-stabilizer such as NaOH or Na₂CO₃ increased the conversion of the starting substance without deactivation of the catalyst.

IT **14172-90-8**

RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydroperoxidn. of cumene derivs.)

RN 14172-90-8 HCAPLUS

CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX
NAME)



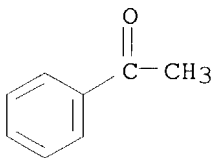
IT **98-86-2P**, preparation **122-00-9P** **617-94-7P**

1197-01-9P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in isopropylbenzene hydroperoxidn.)

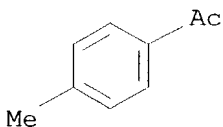
RN 98-86-2 HCAPLUS

CN Ethanone, 1-phenyl- (9CI) (CA INDEX NAME)



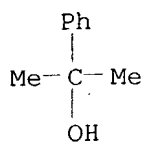
RN 122-00-9 HCAPLUS

CN Ethanone, 1-(4-methylphenyl)- (9CI) (CA INDEX NAME)

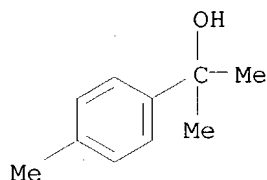


RN 617-94-7 HCAPLUS

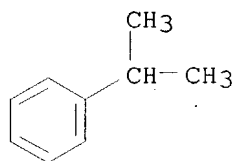
CN Benzenemethanol, α,α-dimethyl- (9CI) (CA INDEX NAME)



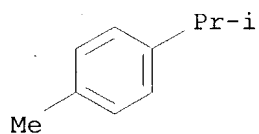
RN 1197-01-9 HCAPLUS
CN Benzenemethanol, $\alpha,\alpha,4$ -trimethyl- (9CI) (CA INDEX NAME)



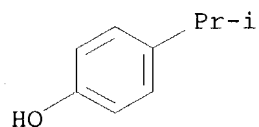
IT 98-82-8 99-87-6 99-89-8 100-18-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroperoxidn. of, catalysts for)
RN 98-82-8 HCAPLUS
CN Benzene, (1-methylethyl)- (9CI) (CA INDEX NAME)



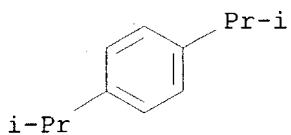
RN 99-87-6 HCAPLUS
CN Benzene, 1-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 99-89-8 HCAPLUS
CN Phenol, 4-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 100-18-5 HCAPLUS
CN Benzene, 1,4-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



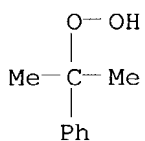
IT 80-15-9P 98-49-7P 3077-71-2P

3159-98-6P 23074-45-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

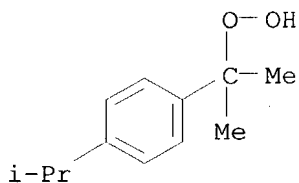
RN 80-15-9 HCAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



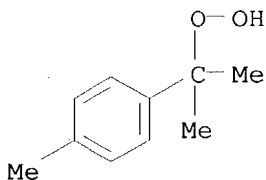
RN 98-49-7 HCAPLUS

CN Hydroperoxide, 1-methyl-1-[4-(1-methylethyl)phenyl]ethyl (9CI) (CA INDEX NAME)



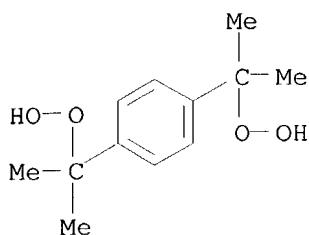
RN 3077-71-2 HCAPLUS

CN Hydroperoxide, 1-methyl-1-(4-methylphenyl)ethyl (9CI) (CA INDEX NAME)

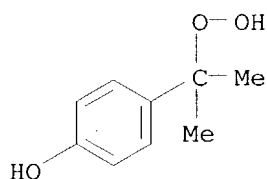


RN 3159-98-6 HCAPLUS

CN Hydroperoxide, [1,4-phenylenebis(1-methylethylidene)]bis- (9CI) (CA INDEX NAME)



RN 23074-45-5 HCAPLUS
 CN Phenol, 4-(1-hydroperoxy-1-methylethyl)- (9CI) (CA INDEX NAME)



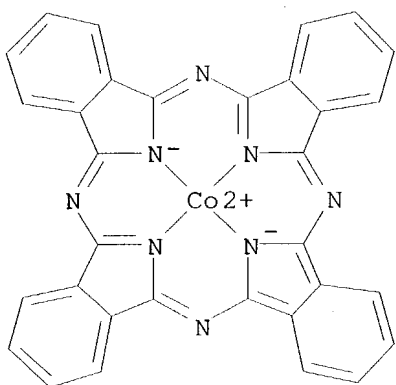
L43 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1975:170383 HCAPLUS
 DOCUMENT NUMBER: 82:170383
 TITLE: Catalysts for oxidizing phenols to quinones
 INVENTOR(S): Omura, Yoshiaki; Nakamura, Michihiro; Oka, Masanari;
 Fujiwara, Yuzuru; Itoi, Kazuo
 PATENT ASSIGNEE(S): Kuraray Co., Ltd.
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|--------------|
| JP 49127937 | A2 | 19741207 | JP 1973-44899 | 19730419 <-- |
| JP 56041611 | B4 | 19810929 | | |

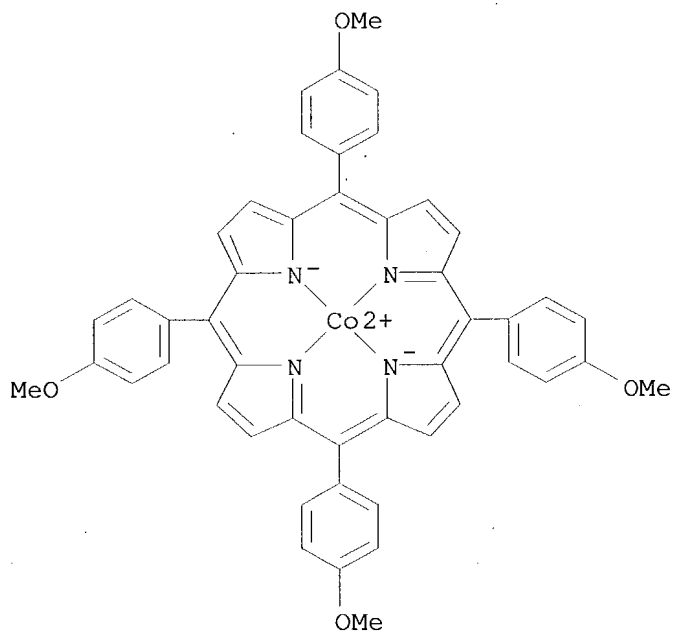
PRIORITY APPLN. INFO.: JP 1973-44899 19730419 <--
 AB Phenols were oxidized to quinones with air or O with an organic Co complex containing N-compound ligands. Thus, O was introduced at 20° for 5 hr to 10 g 2,3,6-trimethylphenol and 0.5 g tetraphenylporphyrin Co complex in 200 ml C6H6 to give 8.9 g 2,3,6-trimethylbenzoquinone. Similarly, 2,4,6- and 3,4,5-trimethylphenol were oxidized to 2,4,6- and 3,4,5-trimethyl-4-hydroxycyclohexa-2,5-dienone, resp. Dimethylglyoxime-pyridine Co complex, phthalocyanine Co complex, or tetra(p-chloro- or methoxyphenyl)porphyrin Co complex was also the catalyst.

IT **3317-67-7 28903-71-1 55915-17-8**
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, for oxidation of phenols to quinones)

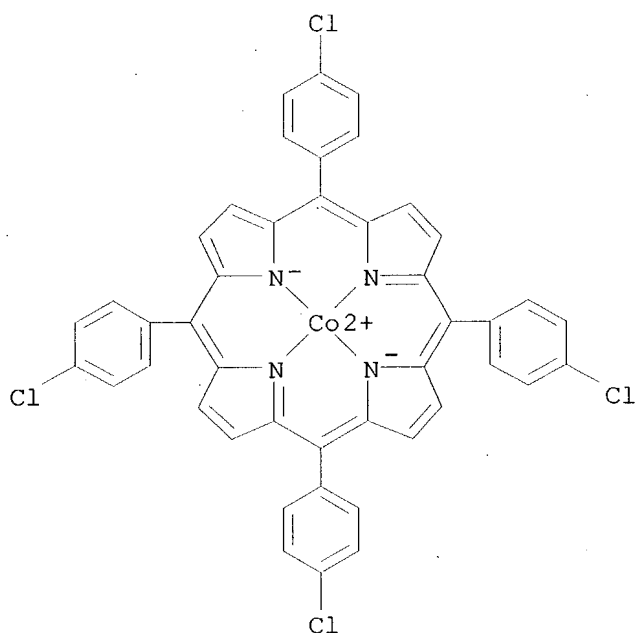
RN 3317-67-7 HCAPLUS
 CN Cobalt, [29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,.ka
 ppa.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



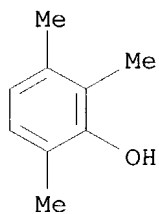
RN 28903-71-1 HCAPLUS
 CN Cobalt, [5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



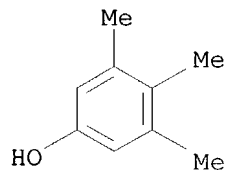
RN 55915-17-8 HCAPLUS
 CN Cobalt, [5,10,15,20-tetrakis(4-chlorophenyl)-21H,23H-porphinato(2-)-
 κ N21, κ N22, κ N23, κ N24]-, (SP-4-1)- (9CI) (CA INDEX
 NAME)



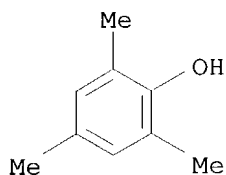
IT 2416-94-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation to trimethylbenzoquinone, cobalt complex catalysts for)
 RN 2416-94-6 HCAPLUS
 CN Phenol, 2,3,6-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



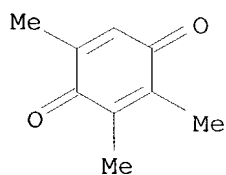
IT 527-54-8 527-60-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation to trimethylhydroxycyclohexadienone)
 RN 527-54-8 HCAPLUS
 CN Phenol, 3,4,5-trimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



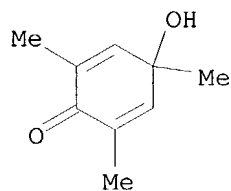
RN 527-60-6 HCAPLUS
 CN Phenol, 2,4,6-trimethyl- (9CI) (CA INDEX NAME)



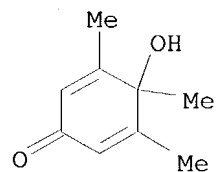
IT 935-92-2P 16404-66-3P 55776-84-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 935-92-2 HCAPLUS
 CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5-trimethyl- (9CI) (CA INDEX NAME)



RN 16404-66-3 HCAPLUS
 CN 2,5-Cyclohexadien-1-one, 4-hydroxy-2,4,6-trimethyl- (6CI, 7CI, 8CI, 9CI)
 (CA INDEX NAME)



RN 55776-84-6 HCAPLUS
 CN 2,5-Cyclohexadien-1-one, 4-hydroxy-3,4,5-trimethyl- (9CI) (CA INDEX NAME)



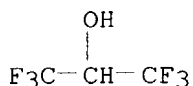
=> d ibib abs hitstr 124 1-2

L24 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:730665 HCAPLUS
DOCUMENT NUMBER: 135:272550
TITLE: Modifying chemoselectivity during oxidation of
nitrogen compounds
INVENTOR(S): **Bernardelli, Patrick**
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

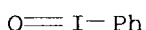
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|------------------|----------|
| WO 2001072667 | A2 | 20011004 | WO 2001-EP3635 | 20010322 |
| WO 2001072667 | A3 | 20011213 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| FR 2807032 | A1 | 20011005 | FR 2000-3991 | 20000329 |
| FR 2807032 | B1 | 20030418 | | |
| EP 1268366 | A2 | 20030102 | EP 2001-929478 | 20010322 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | |
| BR 2001009551 | A | 20030610 | BR 2001-9551 | 20010322 |
| JP 2003528834 | T2 | 20030930 | JP 2001-570583 | 20010322 |
| US 2003176723 | A1 | 20030918 | US 2003-240364 | 20030227 |
| PRIORITY APPLN. INFO.: | | | FR 2000-3991 A | 20000329 |
| | | | WO 2001-EP3635 W | 20010322 |
| OTHER SOURCE(S): | CASREACT 135:272550 | | | |
| AB | The invention concerns a method for chemoselective oxidation of an organic compound comprising several potentially oxidizable groups whereof at least one is a nitrogen group. Said method is characterized in that it consists in using at least a protic solvent, which is a good donor of hydrogen bonds, enabling limitation of N-oxidation E.g., oxidation of N-(9-methyl-4-oxo-1-phenyl-3,4,6,7-tetrahydro[1,4]diazepino[6,7,1-hi]indol-3-yl)isonicotinamide by iodosylbenzene catalyzed by tetra(2,6-dichlorophenyl)porphyrin manganese gave a mixture of six products. Use of (CF ₃) ₂ CHOH/PhCF ₃ as solvent decreased the yield of the N-oxide product. | | | |
| IT | 75-89-8, 2,2,2-Trifluoroethanol 920-66-1 | | | |
| RL: | NUU (Other use, unclassified); USES (Uses) (chemoselective oxidation of nitrogen compds.) | | | |
| RN | 75-89-8 HCAPLUS | | | |
| CN | Ethanol, 2,2,2-trifluoro- (6CI, 8CI, 9CI) (CA INDEX NAME) | | | |

F₃C-CH₂-OH

RN 920-66-1 HCAPLUS
 CN 2-Propanol, 1,1,1,3,3,3-hexafluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 536-80-1, Iodosylbenzene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chemoselective oxidation of nitrogen compds.)
 RN 536-80-1 HCAPLUS
 CN Benzene, iodosyl- (9CI) (CA INDEX NAME)



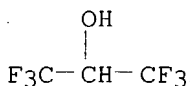
L24 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2001:115086 HCAPLUS
 DOCUMENT NUMBER: 134:178573
 TITLE: Process for the metalloporphyrin **catalyzed**
 oxidation of organic compounds
 INVENTOR(S): **Bernardelli, Patrick**
 PATENT ASSIGNEE(S): Warner Lambert Company, USA
 SOURCE: PCT Int. Appl., 20 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2001010797 | A1 | 20010215 | WO 2000-EP7726 | 20000809 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| BR 2000013018 | A | 20020416 | BR 2000-13018 | 20000809 |
| EP 1208069 | A1 | 20020529 | EP 2000-960420 | 20000809 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| JP 2003506419 | T2 | 20030218 | JP 2001-515270 | 20000809 |
| ZA 2002000130 | A | 20030407 | ZA 2002-130 | 20020107 |
| PRIORITY APPLN. INFO.: | | | US 1999-148079P | P 19990810 |
| | | | US 1999-150101P | P 19990820 |
| | | | WO 2000-EP7726 | W 20000809 |

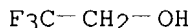
OTHER SOURCE(S): CASREACT 134:178573
 AB An organic compound (e.g., Diazepam) is oxidized using a catalytic amount of metalloporphyrin (tetrakis(pentafluorophenyl)porphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, aprotic, polyhalogenated solvent (benzotrifluoride). Oxidation of

diazepam is conducted to mimic oxidation (metabolism) in biol. systems. The products of the oxidation of diazepam are separated and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert aprotic solvent shows improved oxidation yields when compared to prior art (e.g., CH₃CN-CH₂Cl₂-water mixts.).

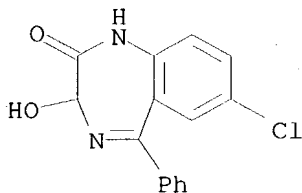
IT **920-66-1**, 1,1,1,3,3,3-Hexafluoro-2-propanol
 RL: CAT (Catalyst use); USES (Uses)
 (co-solvent; process for metalloporphyrin-**catalyzed** oxidation of organic compds.)
 RN 920-66-1 HCAPLUS
 CN 2-Propanol, 1,1,1,3,3,3-hexafluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)



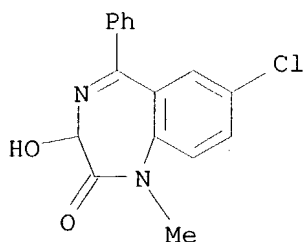
IT **75-89-8**, 2,2,2-Trifluoroethanol
 RL: NUU (Other use, unclassified); USES (Uses)
 (co-solvent; process for metalloporphyrin-**catalyzed** oxidation of organic compds.)
 RN 75-89-8 HCAPLUS
 CN Ethanol, 2,2,2-trifluoro- (6CI, 8CI, 9CI) (CA INDEX NAME)



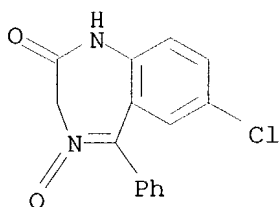
IT **604-75-1P 846-50-4P 963-39-3P**
1088-11-5P 2888-64-4P 4797-43-7P,
 6-Chloro-4-phenyl-2-(1H)-quinazolinone **20927-53-1P**,
 6-Chloro-4-phenyl-1-methyl-2-(1H)-quinazolinone
 RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (process for metalloporphyrin-**catalyzed** oxidation of organic compds.)
 RN 604-75-1 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



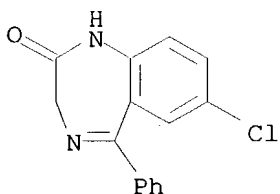
RN 846-50-4 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



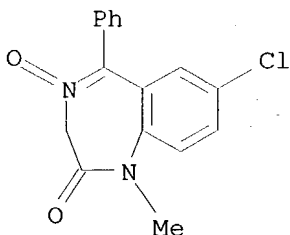
RN 963-39-3 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-, 4-oxide (7CI, 8CI, 9CI) (CA INDEX NAME)



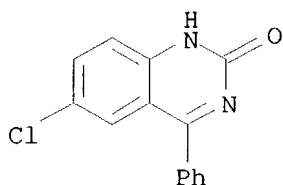
RN 1088-11-5 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl- (8CI, 9CI) (CA INDEX NAME)



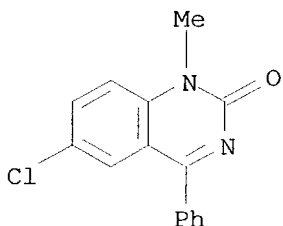
RN 2888-64-4 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-, 4-oxide (7CI, 8CI, 9CI) (CA INDEX NAME)



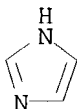
RN 4797-43-7 HCAPLUS
 CN 2(1H)-Quinazolinone, 6-chloro-4-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 20927-53-1 HCAPLUS
CN 2(1H)-Quinazolinone, 6-chloro-1-methyl-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



IT 288-32-4, Imidazole, uses 1119-94-4,
Dodecyltrimethylammonium bromide 79968-43-7
RL: CAT (Catalyst use); USES (Uses)
(process for metalloporphyrin-catalyzed oxidation of organic
compds.)
RN 288-32-4 HCAPLUS
CN 1H-Imidazole (9CI) (CA INDEX NAME)

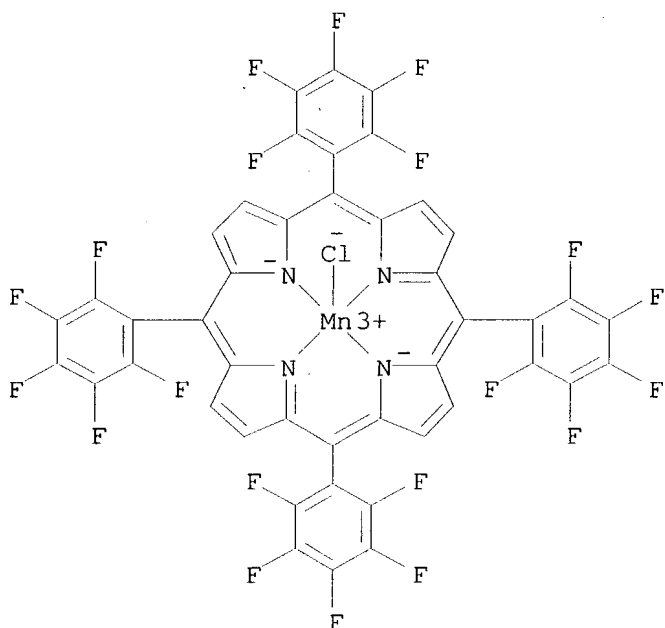


RN 1119-94-4 HCAPLUS
CN 1-Dodecanaminium, N,N,N-trimethyl-, bromide (9CI) (CA INDEX NAME)

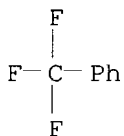
$\text{Me}_3^+\text{N}^-(\text{CH}_2)_{11}-\text{Me}$

● Br^-

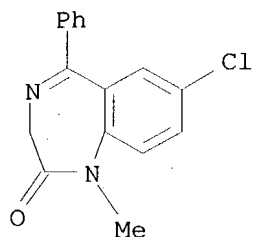
RN 79968-43-7 HCAPLUS
CN Manganese, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-
porphinato(2-)- $\kappa\text{N}21,\kappa\text{N}22,\kappa\text{N}23,\kappa\text{N}24$]-, (SP-5-12)-
(9CI) (CA INDEX NAME)



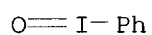
IT **98-08-8**, Benzotrifluoride
 RL: NUU (Other use, unclassified); USES (Uses)
 (process for metalloporphyrin-**catalyzed** oxidation of organic
 compds.)
 RN 98-08-8 HCAPLUS
 CN Benzene, (trifluoromethyl)- (9CI) (CA INDEX NAME)



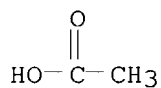
IT **439-14-5**, Diazepam **536-80-1**, Iodosylbenzene
631-61-8, Ammonium acetate **7722-84-1**, Hydrogen peroxide,
 reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process for metalloporphyrin-**catalyzed** oxidation of organic
 compds.)
 RN 439-14-5 HCAPLUS
 CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl- (8CI,
 9CI) (CA INDEX NAME)



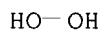
RN 536-80-1 HCAPLUS
CN Benzene, iodosyl- (9CI) (CA INDEX NAME)



RN 631-61-8 HCAPLUS
CN Acetic acid, ammonium salt (8CI, 9CI) (CA INDEX NAME)



RN 7722-84-1 HCAPLUS
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT